CSE 599d - Quantum Computing
Mixed Quantum States and Open Quantum Systems

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So far we have been dealing with quantum states which are what are known as *pure* quantum states. Here *pure* refers to the fact that our description of the system is entirely quantum mechanical. But we saw when we were discussing our information processing machines, that there were these equally valid probabilistic machines that had their own equally valid formulation. Is there a way to include the latter within the confines of the former and in particular to mix quantum descriptions with classical descriptions? This leads us to what are known as *mixed* quantum states which we will discuss in this lecture.

Another reason to care about mixed quantum states is to deal with the case where we have only part of a quantum system. Thus, for instance, we may have the entangle two qubit state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Now of course we can always figure out what quantum theory predict for our half of this quantum system by just acknowledging that this is the true description of the quantum system. But often it is convenient to discuss just one half of this quantum state, i.e. we are looking for a description of one of the two qubits for this state. It is important to realize that we must always use such descriptions appropriately: just because our description of one half is different than that of the whole does not mean that the state has changed in any way! It will turn out that the appropriate way to discuss quantum systems like this is to again consider mixed quantum states.

I. MIXED STATES AND DENSITY OPERATORS

Suppose I set up the following situation. With probability p I prepare a quantum system into a state with the description $|\psi_0\rangle$ and with probability $1-p$ I prepare a quantum system into a state with the description $|\psi_1\rangle$. Now of course we could always keep around the above words describing this situation. But this seems like a lot of work. Is there a better way to keep track of all future predictions we can make on such a system? More generally suppose that I prepare state $|\psi_i\rangle$ with probability p_i. Certainly I could keep those words as my description of the quantum system, but there is a better way. We call a setting where we prepare state $|\psi_i\rangle$ with probability p_i an ensemble of pure states. Such ensembles are described by density operator (often called a density operator.) In particular for the above ensemble, the density operator is given by

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{1}$$

where $p_i \geq 0$ and $\sum_i p_i = 1$. Notice that if we have a single pure state, $|\psi\rangle$, then $\rho = |\psi\rangle\langle\psi|$ is just a projector onto this state. Further note that ρ is Hermitian and is also positive. Finally we note that the trace of ρ is unity:

$$\mathrm{Tr}[\rho] = \sum_x \langle x|\rho|x\rangle = \sum_x \langle x| \sum_i p_i |\psi_i\rangle\langle\psi_i||x\rangle = \sum_i p_i \sum_x |\langle\psi_i|x\rangle|^2 = \sum_i p_i = 1 \tag{2}$$

In fact we can show that any matrix which is positive (and hence necessarily hermitian) and has trace unity represents and ensemble of pure states. To see this note that since such a density matrix is positive, there is a basis where it is diagonal and $\sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ with $\lambda_i \geq 0$. But since the trace of this matrix is 1, this implies that $\sum_i \lambda_i = 1$. Thus for such a density matrix we can associate the ensemble which has state $|\psi_i\rangle$ with probability λ_i.

Notice that there is also an ambiguity in what ensemble actually corresponds to a particular density matrix. For example if we have the density matrix for a qubit which corresponds to $|0\rangle$ with 1/2 probability and $|1\rangle$ with 1/2 probability, then this is the same as the density matrix which corresponds to $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ with probability 1/2 and $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ with probability 1/2. In the first case we calculate,

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \tag{3}$$

and in the second case we calculate

$$\sigma = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \tag{4}$$

How do we interpret this ambiguity? Well we will see that for two ensembles which give the same density matrix, then when we use these density matrices will make the same predictions about the future evolution of the quantum system, *assuming* that no information about which ensemble was being used, is involved in the future evolution. This means that we have to be careful about the situation where information about the ensemble becomes involved in the our protocols, but if this doesn't happen, then the density matrix is all that we will need.

Rule 1 Mixed State Version: (Configuration Description) Our quantum information processing machine again has a finite set of configurations, described by elements from some alphabet Σ. But now instead of our description being a unit vector of complex numbers of size $|\Sigma|$, our description is given by a positive trace one operator on $\mathbb{C}^{|\Sigma|}$, which we call a density operator or density matrix.

Okay so we've redefined Rule 1. How do the other rules change? By the end of all of this we will have gone through even more versions of the following rules. But now let's look at Rule 2. In Rule 2 for pure states, we said that evolution was described by a unitary matrix U such that if the initial description was the pure state $|\psi\rangle$, then the description after this evolution was given by $U|\psi\rangle$. So how do we modify this for mixed states. Well if we have an ensemble $\{p_i, |\psi_i\rangle\}$, then certainly each $|\psi_i\rangle$ will evolve according to Rule 2. So this means that if the initial ensemble is $\{p_i, |\psi_i\rangle\}$ then the ensemble after such unitary evolution will be $\{p_i, U|\psi_i\rangle\}$. This means that the initial mixed state is $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ and the mixed state after evolution is $\rho' = \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger$. Or in other words, $\rho' = U\rho U^\dagger$. Thus we have the following modified Rule 2:

Rule 2 Mixed State Version: (Evolution) Evolution of the N configuration system is described by a $N \times N$ unitary matrix. If the initial mixed state before the unitary evolution was ρ, then the mixed state after the evolution is given by

$$\rho' = U\rho U^\dagger \tag{5}$$

Next onward to Rule 3, measurement. Recall that our latest version of the measurement rule for pure states says that a measurement on a N configuration systems is described by N orthogonal projectors P_j. The probability of obtaining outcome j given that the state is $|\psi\rangle$ was then $Pr(j) = \langle\psi|P_j|\psi\rangle$ and the new state was $|\psi'\rangle = P_j|\psi\rangle/\sqrt{Pr(j)}$. How will this change for our mixed states? Well the probability that we observe outcome j is given by the probability that we observe outcome j given that the pure state was $|\psi_i\rangle$ times the probability that the pure state we had was $|\psi_i\rangle$. Or, in equationese,

$$Pr(j) = \sum_i p_i \langle\psi_i|P_j|\psi_i\rangle \tag{6}$$

Now if we insert an identity operator $I = \sum_{k=0}^{N-1} |k\rangle\langle k|$ into this expression at the write point, we can rewrite this as

$$Pr(j) = \sum_i p_i \langle\psi_i|P_j \sum_{k=0}^{N-1} |k\rangle\langle k|\psi_i\rangle = \sum_i p_i \sum_{k=0}^{N-1} \langle k|\psi_i\rangle\langle\psi_i|P_j|k\rangle = \sum_{k=0}^{N-1} \langle k| \sum_i p_i |\psi_i\rangle\langle\psi_i|P_j|k\rangle = \sum_{k=0}^{N-1} \langle k|\rho P_j|k\rangle \tag{7}$$

or, recalling that the trace is the sum of the diagonal elements of a matrix:

$$Pr(j) = \mathrm{Tr}[\rho P_j] \tag{8}$$

The trace is cyclic, $\mathrm{Tr}[AB] = \mathrm{Tr}[BA]$, so this is also equal to $\mathrm{Tr}[P_j\rho]$.

How does the state change? Well, given each state $|\psi_i\rangle$ changes to $P_j|\psi_i\rangle/\sqrt{Pr[j]}$, we can express the new density matrix after the measurement, given outcome j as

$$\rho' = \sum_i p_i \frac{P_j|\psi_i\rangle}{\sqrt{Pr[j]}} \frac{\langle\psi_i|P_j^\dagger}{\sqrt{Pr[j]}} = \frac{P_j \sum_i p_i |\psi_i\rangle\langle\psi_i|P_j}{Pr[j]} = \frac{P_j\rho P_j}{Pr[j]} \tag{9}$$

Rule 3 Mixed State Version: A measurement is described by a set of orthogonal projectors P_j. The probability of observing outcome j given that the initial state is the mixed state ρ is $\mathrm{Tr}[P_j\rho]$. Given that we observe outcome j, the new mixed state is given by

$$\rho' = \frac{P_j\rho P_j}{Pr[j]} \tag{10}$$

Finally we can ask about what happens when we combine two systems together. This rule isn't much changed: now instead of the new pure state living in $\mathbb{C}^N \times \mathbb{C}^M$, it is a matrix which operates on $\mathbb{C}^N \times \mathbb{C}^M$. This isn't so different, so we won't formally express it and hopefully by now you are getting very used to tensor products.

II. HALF AN ENTANGLED STATE

Okay so we have defined our new rules for mixed states. What else do we need mixed states for? In this section we will describe another reason, and perhaps the most interesting reason, to use mixed states.

Suppose that we have two qubits which have the quantum state $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle)$. As we've explained before, there is no way to express this as $|\psi\rangle = |a\rangle \otimes |b\rangle$ where $|a\rangle$ is the quantum state for the first qubit and $|b\rangle$ is the quantum state for the second qubit. Okay, fine, we need to keep around this whole description if we want to be sure that everything that is done to both qubits can be predicted.

But now consider the following situation. Suppose that there are two qubits in the entangled quantum state $|\psi\rangle = \alpha|0\rangle \otimes |0\rangle + \beta|1\rangle \otimes |1\rangle$. Now suppose that we measure the first qubit with the projection operators P_0 and P_1. Then the probability of getting outcome 0 is

$$\begin{aligned} Pr(0) &= \langle\psi|P_0 \otimes I|\psi\rangle = (\alpha^*\langle 0| \otimes \langle 0| + \beta^*\langle 0| \otimes \langle 0|)P_0 \otimes I(\alpha|0\rangle \otimes |0\rangle + \beta|1\rangle \otimes |1\rangle) \\ &= |\alpha|^2\langle 0|P_0|0\rangle + |\beta|^2\langle 1|P_0|1\rangle, \end{aligned} \tag{11}$$

and the probability of getting outcome 1 is likewise

$$Pr(1) = |\alpha|^2\langle 0|P_1|0\rangle + |\beta|^2\langle 1|P_1|1\rangle. \tag{12}$$

Notice, however that if we set

$$\rho = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1| \tag{13}$$

then this would also yield the correct expressions:

$$Pr(0) = \mathrm{Tr}[P_0\rho], \quad Pr(1) = \mathrm{Tr}[P_1\rho]. \tag{14}$$

Suppose that a unitary U_A was applied to the first qubit before this rotation, then the probability of getting outcome 0 is

$$\begin{aligned} Pr(0) &= \langle\psi|(U_A^\dagger \otimes I)P_0 \otimes I(U_A \otimes I)|\psi\rangle = (\alpha^*\langle 0| \otimes \langle 0| + \beta^*\langle 0| \otimes \langle 0|)(U_A^\dagger P_0 U_A) \otimes I(\alpha|0\rangle \otimes |0\rangle + \beta|1\rangle \otimes |1\rangle) \\ &= |\alpha|^2\langle 0|U_A^\dagger P_0 U_A|0\rangle + |\beta|^2\langle 1|U_A^\dagger P_0 U_A|1\rangle = \mathrm{Tr}[U_A\rho U_A^\dagger P_0], \end{aligned} \tag{15}$$

Thus we see that unitary evolution of the first qubit corresponds to unitary evolution of the ρ. Further we can show that whatever we do to the second qubit, all our predictions (measurement probabilities, new states) will be unaffected.

Now let's generalize this and give it a name. Suppose that we have a bipartite quantum system with Hibert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Suppose the state of this full bipartite quantum system is $|\psi\rangle \in \mathcal{H}$. Then this corresponds to the density matrix on this full space of $\rho = |\psi\rangle\langle\psi|$. We then define the *reduced* density matrix for system A as

$$\rho_A = \mathrm{Tr}_B[\rho] = \sum_{i=1}^{\dim\mathcal{H}_B} \langle\phi_i|_B\rho|\phi_i\rangle_B \tag{16}$$

where this summation is over a basis for $\mathcal{H}_B$, $|\phi_i\rangle_B$. It is important to realize that $\langle\phi_i|\rho|\phi_i\rangle$ is not a scalar but is instead a $\dim\mathcal{H}_A$ dimensional density matrix. As an example, consider two qubits in the state $|\psi\rangle = \frac{1}{2}|0\rangle \otimes |0\rangle + \frac{\sqrt{3}}{2}|1\rangle \otimes |1\rangle$. Then

$$\rho_A = \sum_{x=0}^{1}\langle 0|_B\left(|\psi\rangle\langle\psi|\right)|0\rangle_B \tag{17}$$

Now $\langle 0|_B|\psi\rangle = \langle 0|_B\left(\frac{1}{2}|0\rangle \otimes |0\rangle + \frac{\sqrt{3}}{2}|1\rangle \otimes |1\rangle\right) = \frac{1}{2}|0\rangle\langle 0|0\rangle + \frac{\sqrt{3}}{2}|1\rangle\langle 0|1\rangle = \frac{1}{2}|0\rangle$. Similar expressions lead us to

$$\rho_A = \frac{1}{4}|0\rangle\langle 0| + \frac{3}{4}|1\rangle\langle 1| \tag{18}$$

It is also useful to note that if we take the partial trace of a separable pure state $|\psi\rangle \otimes |\phi\rangle$, then this just gives us the mixed state representation corresponding to the appropriate subsystem's pure state: $\rho_A = |\psi\rangle\langle\psi|$.

The reduced trace operation is a very useful tool: it allows us to discuss half of an entangled state. Just as long as we don't know things like measurement outcomes on the other half of the entangled state, or evolution on the full entangled state, then the reduced density matrix contains everything we'll ever need.

Notice also that we have moved into a new realm here. Now, no longer are we dealing with single isolated quantum system, but we are obtaining tools for talking about quantum subsystems which interact with other quantum subsystems but we only have access to one of the subsystems (or are only interested in it's dynamics.) The study of such *open quantum systems* is of vital importance in real world physics because most quantum systems do interact strongly with other quantum systems and are hard to isolate. We'll have more to say about this latter.

III. PURIFICATIONS

In the previous section we saw that half of an entangled state could be represented by a mixed state. A natural question to ask is whether all mixed states can be represented as a pure state on a larger system. The answer to this question is yes. Let's see how to do this. Suppose that have the mixed state ρ which we can spectrally decompose as $\rho = \sum_{i=1}^{\dim\mathcal{H}} p_i |\psi_i\rangle\langle\psi_i|$ for some orthogonal $|\psi\rangle$ (some of the p_i may be zero.) Now append a second subsystem which has a Hilbert space the same dimension the original subsystem, $\dim\mathcal{H}_B = \dim\mathcal{H}$. Then consider the following state

$$|\psi\rangle = \sum_{i=1}^{\dim\mathcal{H}} \sqrt{p_i}|\psi_i\rangle \otimes |\phi_i\rangle \tag{19}$$

where $|\phi_i\rangle$ is some basis for $\mathcal{H}_B$. Then we can calculate the reduced density matrix for this state:

$$\begin{aligned} \mathrm{Tr}_B[|\psi\rangle\langle\psi|] &= \mathrm{Tr}_B\left[\sum_{i=1}^{\dim\mathcal{H}} \sqrt{p_i}|\psi_i\rangle \otimes |\phi_i\rangle \sum_{j=1}^{\dim\mathcal{H}} \sqrt{p_j}\langle\psi_j| \otimes \langle\phi_j|\right] \\ &= \sum_{i,j=1}^{\dim\mathcal{H}} \sqrt{p_i p_j}|\psi_i\rangle\langle\psi_j| \mathrm{Tr}[|\phi_i\rangle\langle\phi_i|] \\ &= \sum_{i,j=1}^{\dim\mathcal{H}} \sqrt{p_i p_j}|\psi_i\rangle\langle\psi_j|\delta_{ij} = \sum_{i=1}^{\dim\mathcal{H}} p_i|\psi_i\rangle\langle\psi_i| \end{aligned} \tag{20}$$

which is just ρ. Thus we see that we have constructed a *purification* of ρ.

Actually what we've done is we have provided a purification of a particular ensemble interpretation of a density matrix ρ. More generally, consider the density matrix which corresponds to an ensemble of state $|\psi_i\rangle$ drawn with probability p_i. Now append a subsystem which, instead of being the dimension of the original space, has a dimension equal to the number of different states in the ensemble. Then it is easy to check that the state we constructed above, will again be a pure state, which, when traced over the extra subsystem, yields the density matrix corresponding to this ensemble.

Our construction was totally generic, so every mixed state can be thought of as an pure state on a larger Hilbert space. Notice also that our purification was not necessarily unique. We'll return to this in a bit. Purification is an important tool. Why? Because proving things about pure states is often much easier than proving things about mixed states. So in quantum information theory, for example, one constructs purifications all the time, so that one doesn't need to worry about the complications that arise when thinking about mixed states.

IV. WHEN DENSITY MATRICES ARE THE SAME

We saw above an example where two ensembles gave rise to the same density matrix. An interesting question to ask is when this is possible.

Suppose that we purify ρ by the state

$$|\psi\rangle = \sum_{i=1}^{\dim\mathcal{H}} \sqrt{p_i}|\psi_i\rangle \otimes |\phi_i\rangle \tag{21}$$

Suppose that we measure the extra subsystem in the $|\phi_i\rangle$ basis. Then it is easy to calculate that the probability that we observe outcome i is p_i and the resulting state is $|\psi_i\rangle \otimes |\phi_i\rangle$. Thus we see that by measuring in this basis we have realized the ensemble corresponding to choosing $|\psi_i\rangle$ with probability p_i. For a different density matrix σ we can purify by a different state (but living in the same Hilbert space),

$$|\psi\rangle = \sum_{i=1}^{\dim\mathcal{H}} \sqrt{q_i}|\tilde{\psi}_i\rangle \otimes |\tilde{\phi}_i\rangle \tag{22}$$

Measuring in the $|\tilde{\phi}_i\rangle$ basis will them realize an ensemble corresponding to choosing $|\tilde{\psi}_i\rangle$ with probability q_i.

Now what if these density matrices ρ and σ are equal? Suppose we pad the purifications in such a way that the dimension of the extra subsystems are the same and take the appropriate p_i and q_i equal to zero. Now there will be a unitary transform between the two states $|\phi_i\rangle$ and $|\tilde{\phi}_i\rangle$. Thus we see that if we take our first purification and measure in the $|\phi_i\rangle$ basis, then we will obtain the ensemble $\{p_i, |\psi_i\rangle\}$, but if we measure in the basis $U|\phi_i\rangle$, then we will obtain the ensemble $\{q_i, |\tilde{\psi}_i\rangle\}$. Applying this unitary rotation, we see that we can write the second purification as

$$|\psi\rangle = \sum_{i=1}^{\dim\mathcal{H}} \sqrt{q_i}|\tilde{\psi}_i\rangle \otimes U|\phi_i\rangle \tag{23}$$

Express this unitary in the $|\phi_i\rangle$ basis, we obtain

$$U|\phi_i\rangle = \sum_{j=1}^{d} U_{ji}|\phi_j\rangle \tag{24}$$

where d is the larger of the dimensions we choose above. Then

$$|\psi\rangle = \sum_{j=1}^{d}\sum_{i=1}^{\dim\mathcal{H}} U_{ji}\sqrt{q_i}|\tilde{\psi}_i\rangle \otimes |\phi_j\rangle \tag{25}$$

From this expression we see that the the two ensembles $\{p_i, |\psi_i\rangle\}$ and $\{q_i, |\tilde{\psi}_i\rangle\}$ represent the same density matrix if

$$\sqrt{p_i}|\psi_i\rangle = \sum_{j=1}^{d} \sqrt{q_j}U_{ij}|\tilde{\psi}_j\rangle \tag{26}$$

This is known as the unitary degree of freedom in an ensemble.

V. THE BLOCH BALL

When we first encountered qubits, we encountered the Bloch sphere. There every pure state, modulo a global phase choice, could be represented by a point on the unit sphere. There is a useful generalization of this concept for mixed states of a single qubit. This is the notion of the Bloch Ball. Actually it is often called the Bloch sphere as well, because physicists are always messing up the difference between a sphere and ball and mathematicians are always making this discussion (which is one of the reasons they get picked on more during recess.)

A density matrix for a single qubit will be a positive trace one hermitian matrix of size 2×2. We can expand any Hermitian operator on a single qubit as

$$s_I I + s_X X + s_y Y + s_z Z == \begin{bmatrix} s_I + s_Z & s_X + is_Y \\ s_X - is_Y & s_I - s_Z \end{bmatrix} \tag{27}$$

Since the trace of this matrix is 1, and hence the sum of the eigenvalues of this matrix is 1, the only way this matrix can have a negative eigenvalue is if one of these two eigenvalues is negative. This can only happen if the determinant of the matrix is negative. Thus a necessary and sufficient condition for this trace one matrix to be positive is that it's determinant must be positive. The determinant is easily calculated to be

$$(s_I + s_Z)(s_I - s_Z) - (s_X + is_Y)(s_X - is_Y) = s_I^2 - s_Z^2 - s_X^2 - s_Y^2 \tag{28}$$

The requirement that the trace of this matrix is 1 implies that $s_I = \frac{1}{2}$. Thus the requirement that the determinant be positive implies that

$$\frac{1}{4} - s_X^2 - s_Y^2 - s_Z^2 \geq 0 \Rightarrow s_X^2 - s_Y^2 - s_Z^2 \leq \frac{1}{4} \tag{29}$$

Thus we see that a positive trace one hermitian matrix can be represented by a vector of length less than one, $\vec{n}$, $|\vec{n}| \leq 1$, such that

$$\rho = \frac{1}{2}(I + \vec{n} \cdot \sigma) \tag{30}$$

This representation of the ρ is called the Bloch ball representation of a mixed single qubit state.

Where do the pure states lie on the Bloch ball? Recall that the pure states Bloch sphere representation was

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \tag{31}$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$. These pure states have mixed state denisty matrix of

$$\begin{aligned}
\rho &= \left[\cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle\right]\left[\cos\left(\frac{\theta}{2}\right)\langle 0| + e^{-i\phi}\sin\left(\frac{\theta}{2}\right)\langle 1|\right] \\
&= \cos^2\left(\frac{\theta}{2}\right)|0\rangle\langle 0| + \sin^2\left(\frac{\theta}{2}\right)|1\rangle\langle 1| + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left[e^{i\phi}|1\rangle\langle 0| + e^{-i\phi}|0\rangle\langle 1|\right] \\
&= \frac{1}{2}\left[I + \cos\theta Z + \sin\theta\cos\phi X + \sin\theta\sin\phi Y\right] = \frac{1}{2}(I + \hat{n}\cdot\vec{\sigma})
\end{aligned} \tag{32}$$

where $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is the unit direction pointing in the same direction the state pointed on the unit sphere (and $\vec{\sigma} = (X, Y, Z)$ is the vector of Pauli matrices.) Thus we see that the pure states all lie on the surface of the Bloch ball, i.e. this is just the Bloch sphere!

Actually this situation, where density matrices form a convex set and the pure states lie on the boundary of this set is true in general. That is it is clear that every convex combination of density matrices, ρ_1 and ρ_2, i.e. $p\rho_1 + (1-p)\rho_2$, $0 \leq p \leq 1$ is a valid density matrix. Thus it is clear that the set of density matrices for a convex set. Elements of a convex set which cannot be expressed as a convex combination of different elements of the set are called extremal points in this set. The pure states are the extremal points of the set of density matrices. To see this, assume the opposite: assume that there are two density matrices ρ_1 and ρ_2 which and can be combined to produce the state $\rho = |\psi\rangle\langle\psi|$ and that ρ_1 and ρ_2 are not equal to ρ. Then $\rho = p\rho_1 + (1-p)\rho_2$. Take a state orthogonal to ρ, $|\phi\rangle$. Then $\langle\phi|\rho|\phi\rangle = 0$. But this implies $p\langle\phi|\rho_1|\phi\rangle + (1-p)\langle\phi|\rho_2|\phi\rangle = 0$. Assume $p \neq 0$ or 1. Then this is a sum of two nonnegative terms and these terms are positive, so these terms must be zero. That is $\langle\phi|\rho_i|\phi\rangle = 0$. But this must be true for all $|\phi\rangle$, so in fact $\rho = \rho_1 = \rho_2$. In the case where p is 0 or 1, the only way the equation is true is if state is a convex combination of itself and nothing else. Thus we've shown that pure states cannot be expressed as a convex combination of other elements of the set of mixed states. Thus the pure states are the extremal points in the set of density matrices.

VI. OPEN QUANTUM SYSTEM EVOLUTION

Now we have figured out ways to deal with one half of an entangled quantum state, we can also begin to ask about how we deal with one half of a unitary evolution on a bipartite system. For example, suppose that we have a single qubit in some state $|\psi\rangle$ and a second qubit in the state $|0\rangle$. Then we evolve these two qubits according to a two qubit unitary U like a controlled-NOT. This evolution will, in general, result in an entangled state of the two qubits. If we take the partial trace, we can then calculate a reduced density operator for the first qubit. How do we describe this evolution, if we wish to do it solely from the perspective of the first qubit?

We'll work in a fairly general setting. Suppose that we have a bipartite quantum system (made of two subsystems, A and B) which is initially in the state $\rho = \rho_A \otimes \rho_B$, i.e we have assume that the initial state is separable between the two subsystems. Then we evolve the system with the unitary evolution U. The new density matrix will be $U\rho U^\dagger$. Let's derive a nice expression for this evolution, solely from the perspective of the A subsystem. The new density matrix after this evolution for the A subsystem is

$$\rho_A' = \mathrm{Tr}_B[U\rho U^\dagger] = \mathrm{Tr}_B[U(\rho_A \otimes \rho_B)U^\dagger] \tag{33}$$

Now diagonalize the system B density matrix: $\rho_B = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ and evaluate the partial trace:

$$\rho_A' = \mathrm{Tr}_B[U(\rho_A \otimes \sum_i p_i|\psi_i\rangle_B\langle\psi_i|_B)U^\dagger] = \sum_k \langle k|_B U(\rho_A) \otimes \sum_i p_i|\psi_i\rangle_B\langle\psi_i|_B)U^\dagger|k\rangle \tag{34}$$

Then if we define

$$A_{k,i} = \sqrt{p_i}\langle k|U|\psi_i\rangle \tag{35}$$

then the new density matrix is given by

$$\rho'_A = \sum_i \sum_k A_{k,i}\rho_A A_{k,i}^\dagger \tag{36}$$

The two sums over i and k are usually written as one sum, so that the evolution is given by

$$\rho'_A = \sum_s A_s \rho_A A_s^\dagger \tag{37}$$

This representation of the evolution is known as the Kraus representation or the operator sum representation. The operators A_s are sometimes called Kraus operators.

The Kraus operators satisfy a nice relation due to the unitarity of U:

$$\sum_s A_s^\dagger A_s = \sum_i \sum_k \sqrt{p_i}(\langle k|_B U|\psi_i\rangle_B)^\dagger \sqrt{p_i}\langle k|_B U|\psi_i\rangle_B = \sum_i \sum_k p_i \langle\psi_i|_B U|k\rangle_B \langle k|_B U|\psi_i\rangle_B \tag{38}$$

$$\sum_s A_s^\dagger A_s = \sum_i p_i \langle\psi_i|_B U^\dagger U|\psi_i\rangle_B = \sum_i p_i \langle\psi_i|_B I_{AB}|\psi_i\rangle_B = \sum_i p_i I_A = I_A \tag{39}$$

where I_A is the identity operator on subsystem A and I_{AB} is the identity operator on subsystems A and B. Thus we have shown that

$$\sum_s A_s^\dagger A_s = I \tag{40}$$

We have shown that evolutions which begin in separable states and which then proceed via unitary evolution on the bipartite system can all be expressed in the operator sum representation given above. Is the opposite true? Is it true that whenever we have evolution which can be described by the operator sum form, with the proper condition given above, then there will be a unitary evolution and a properly prepared initial state which corresponds to this evolution? The answer is yes!

In fact this motivates us to define our most general evolution description:

Rule 2 Open Quantum Systems Version (Evolution) The evolution of an open quantum system, given that it is initial separable with the other subsystems it is interacting with, has an evolution described the operators A_s which satisfy $\sum_s A_s^\dagger A_s = I$. This evolution on a density matrix ρ results in the new density matrix

$$\rho' = \sum_k A_k \rho A_k^\dagger \tag{41}$$

In fact, this should be the defining rule for evolution in quantum theory in a pragmatic sense. Why? Because, while we think that the evolution of our physical theories is unitary (okay we need to be careful here when discussing quantum field theory, but that withstanding) but in the real world we never observe isolated quantum system which do not interact with any external subsystems. In the real world evolution is always described by Kraus operators. Of course these Kraus operators may be so indistinguishable from unitary evolution that for all effective purposes we have unitary evolution. This is one of the dangers of mixing philosophy and physics. We started out by taking the position that all quantum systems are open quantum systems and so unitary evolution never occurs, but then argued that often times this doesn't matter because this open quantum system evolution looks almost identical to unitary evolution, i.e. that some quantum systems behave for all effective purposes like closed quantum systems. This is the danger, of course of mixing a pragmatic physics with a dewy eyed rigor: we end up running circular arguments into silly places.

VII. GENERALIZED MEASUREMENTS AND POVMS

Now that we have generalized evolutions to open quantum systems, we can ask about generalizing the idea of measurements to open quantum systems (okay this is the last time we'll generalize measurements!) Suppose we perform the following measurement: we take our quantum system, attach an ancilla quantum subsystem in a pure state $|0\rangle$, and the measure the ancilla subsystem projectively in a fixed basis. What will this look like from the perspective of the original quantum system? Well looking over our derivation of the superoperator derivation, we see that if we measure the system in the $|k\rangle_B$ basis, then the probability of getting outcome k is

$$Pr(k) = \mathrm{Tr}\left[(I \otimes |k\rangle_B\langle k|_B)U(\rho_A \otimes |0\rangle\langle 0|)U^\dagger\right] \tag{42}$$

Expanding this trace, we obtain

$$Pr(k) = \sum_i \sum_j \langle i|_A \otimes \langle j|_B (I \otimes |k\rangle_B\langle k|_B)U(\rho_A \otimes |0\rangle\langle 0|)U^\dagger |i\rangle_A \otimes |j\rangle_B \tag{43}$$

which evaluating the inner products over B yeilds

$$Pr(k) = \sum_i \langle i|_A(\langle k|_B)U(\rho_A \otimes |0\rangle\langle 0|)U^\dagger |k\langle_B |i\rangle_A \tag{44}$$

Expressing this in terms of our $A_s = A_{ki}$ operators (and noting that we only have one term in our spectral decomposition of ρ_B,) we find

$$Pr(k) = \sum_i \langle i|_A A_{k0}\rho A_{k0}^\dagger |i\rangle_A = \mathrm{Tr}[A_{k0}\rho_A A_{k0}^\dagger] \tag{45}$$

or using the cyclic property of the trace, and labelling $M_k = A_{k0}$,

$$Pr(k) = \mathrm{Tr}[\rho_A M_k^\dagger M_k] \tag{46}$$

What is the state of the first subsystem after we get measurement outcome k? Well this state is

$$\rho_A' = \frac{(I \otimes |k\rangle_B\langle k|_B)(\rho_A \otimes |0\rangle\langle 0|)(I \otimes |k\rangle_B\langle k|_B)}{\sqrt{Pr[k]}} \tag{47}$$

But this is just the kth term in our partial trace sum, so we see, following that derivation, that this just

$$\rho_A' = \frac{A_{k0}\rho_A A_{k0}^\dagger}{Pr[k]} \tag{48}$$

or, expressed in our M_k operators:

$$\rho_A' = \frac{M_k \rho_A M_k^\dagger}{(\mathrm{Tr}[\rho_A M_k^\dagger M_k])^{\frac{1}{2}}} \tag{49}$$

Thus we can now define our new, general measurement rule.

Rule 3 Open Quantum Systems Version (Measurement) A measurement on a quantum system ρ is described by a set of measurement operators M_k where $\sum_k M_k^\dagger M_k = I$. The probability of obtaining outcome k is then given by

$$Pr[k] = \mathrm{Tr}[\rho M_k^\dagger M_k] \tag{50}$$

Given that outcome k has occurred, the new density matrix is given by

$$\rho' = \frac{M_k \rho M_k^\dagger}{\sqrt{Pr[k]}} \tag{51}$$

Notice that projective measurements which we have described before occur when the M_k are themselves projectors. Projective measurements are a subset of generalized measurements.

Now often times we are only concerned with the probability of a particular generalized measurement and not with how the state changes. In that case it is convenient to work with what are called positive operator valued measurement (POVMs.) This name is a bet heavy handed in our case of a finite dimensional Hilbert space, but it has stuck, so we will continue to use it. Given a generalized measurement with measurement operator M_k, we can construct the following elements $E_k = M_k^\dagger M_k$. Now the E_k must be positive and further they must sum to unity $\sum_k E_k = I$. The probability of observing outcome k is then $Pr[k] = \mathrm{Tr}[\rho E_k]$. Thus in order to describe the measurement *probabilities* we only need to worry about the POVM elements E_k (these elements are sometimes called "effects.") Since often we are interested in only the probabilities, often we only write down the POVM elements and not the measurement operators.

In fact, we can show that any set of positive E_k which sum to identity can be implemented as a measurement operator. To see this note that because E_k is positive, we can define the square root of this operator (if M is positive, then we can express it as $M = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$, $\lambda_i \geq 0$ and then $\sqrt{M} = \sum_i \sqrt{\lambda_i}|\psi_i\rangle\langle\psi_i|$.) Then if we define $M_k = \sqrt{E_k}$, we see that this is a valid measurement operator: $\sum_k M_k^\dagger M_k = \sum_k \sqrt{E_k}^\dagger \sqrt{E_k} = \sum_k E_k = I$. Thus we see that every set of positive operators which sum to identity can be implemented as a measurement operator.

VIII. COHERENCE AND INTERFERENCE

Finally let's remark about why we are studying open quantum systems. A natural question to ask is what is the difference between the pure state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and the mixed state $\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}I$. Well suppose we apply our friend the Hadamard H to either of these states. In the first case we obtain

$$H\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |0\rangle. \tag{52}$$

In the second case we obtain

$$H\frac{1}{2}IH = \frac{1}{2}H^2 = \frac{1}{2}I. \tag{53}$$

Thus in the first case these amplitudes can interfere and produce the state $|0\rangle$ whereas in the second case the states cannot interfere, because they are in an *incoherent* mixture of the two states.

And this is why we are interested in open quantum systems. Open quantum systems can produce evolution which starts out in a pure state and evolves into a mixed state. Such evolution can destroy our quantum computation. In coming lectures we will discuss such effects, known as decoherence, and this will eventually lead us to the second great discovery of the age of quantum information: quantum error correction (well second for us in this course, at least.)