This lecture studies some examples of the density matrix formalism for quantum statistical mechanics. We will see that the familiar singlet state of two particles has a property known as “entanglement” that is quite surprising from a classical point of view. Entanglement is one of the basic notions of “quantum information”.

Lightning review of the density matrix formalism:

The density operator is explicitly written as

$$\rho = \sum_{\alpha=1}^{N} |\alpha\rangle W_\alpha \langle \alpha|,$$

where $|\alpha\rangle$ are some normalized states (not necessarily orthogonal or complete). This is now shown to reproduce the sort of statistical average discussed above. Let’s take an operator $A$ and ask about its statistical expectation. In a particular orthonormal basis, the matrix representation of $\rho$ is

$$\rho_{n,n'} = \langle n|\rho|n'\rangle = \sum_{\alpha=1}^{N} \langle n|\alpha\rangle \langle \alpha|n'\rangle W_\alpha.$$

Now

$$\text{Tr} \rho A = \sum_{n,n'} \rho_{n,n'} A_{n',n} = \sum_{n,n',\alpha} \langle n|\alpha\rangle \langle \alpha|n'\rangle W_\alpha \langle n'|A|n\rangle.$$

We can simplify this greatly using the completeness relation for the basis $|n\rangle$: completeness requires

$$\sum_{n} |n\rangle \langle n| = 1.$$

Then in the above sum, both the sums over $n$ and $n'$ just give unity, leaving

$$\text{Tr} \rho A = \sum_{\alpha} W_\alpha \langle \alpha|A|\alpha\rangle.$$

Some simple properties of the density matrix that follow from the above definition are

$$\text{Tr} \rho = 1$$

and all diagonal elements are nonnegative, since the diagonal elements are just the probabilities of being in different pure states. We also showed that for a pure state, $\rho^2 = \rho$.

You might ask, given the density matrix, how to express the entropy of a quantum system. The logical definition is the von Neumann entropy, defined (if we want to count entropy dimensionlessly, in “bits”) as

$$S(\rho) = -\text{Tr} \rho \log_2 \rho.$$

For a diagonal density matrix with equal probabilities (this is a mixed state) this reduces to the classical entropy up to a constant. Any pure quantum mechanical state has entropy 0, since a pure state can be converted by a change of basis to a matrix with diagonal elements $1, 0, \ldots, 0$. 
This is connected to some recent developments in the theory of “entanglement” of quantum systems. Suppose that a quantum system is made up of two subsystems $A$ and $B$, and that the whole system $AB$ is in a pure state

$$\rho = |\psi\rangle\langle\psi|.$$  \hfill{(8)}

More precisely, the full system’s Hilbert space is a product of $A$ and $B$ Hilbert spaces. We can define the reduced density matrix for subsystem $A$ by a partial trace over subsystem $B$:

$$\langle \phi_1 | \rho_A | \phi_2 \rangle = \sum_j (\langle \phi_1 | \times \langle \psi_j |) \langle \psi | (| \phi_2 \rangle \times | \psi_j \rangle).$$  \hfill{(9)}

Here the sum is over a basis of the $B$ Hilbert space. This reduced density matrix can give us the results of any measurement of an operator that is of the form $\hat{O}_A \otimes 1_B$, i.e., that can be thought of a measurement on subsystem $A$. To see this, first note that

$$\langle (\hat{O}_A \otimes 1_B) \rangle = \langle \psi | (\hat{O}_A \otimes 1_B) | \psi \rangle = \sum_{i,j} \langle \psi | (| \phi_i \rangle \otimes | \phi_j \rangle) (\langle \phi_i | \otimes \langle \phi_j |) (\hat{O}_A \otimes 1_B) (| \phi_i \rangle \otimes | \phi_j \rangle | \psi \rangle.$$  \hfill{(10)}

Here in the second step we have inserted a version of the identity operator, made from the product basis states; recall that for an orthonormal basis $\sum_k |k\rangle\langle k| = 1$. Applying the same process again to insert another copy of the identity operator, we get

$$\sum_{i,j,k,l} \langle \psi | (| \phi_i \rangle \otimes | \phi_j \rangle) (\langle \phi_i | \otimes \langle \phi_j |) (\hat{O}_A \otimes 1_B) (| \phi_k \rangle \otimes | \phi_l \rangle) (\langle \phi_k | \otimes \langle \phi_l |) | \psi \rangle = \sum_{i,k} \hat{O}_{ik} \rho_{ik} = \text{Tr}(\hat{O}_A \rho_A).$$  \hfill{(11)}

where we have dropped the $A$ and $B$ subscripts in the middle equations.

Note that this can be a mixed density matrix even if we started from a pure state for the whole system. As an example, consider the singlet state $|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle / \sqrt{2}$ for a state of two spin-half particles. The reduced density matrix for either particle is found to be

$$\rho_A = \rho_B = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$  \hfill{(12)}

We can confirm by a calculation (do calculation for singlet) that this gives 0 for a product state $|\psi\rangle = |\psi_1\rangle_1 |\psi_2\rangle_2$, and 1 for a fully entangled state of two qubits (“quantum bits”, i.e., quantum two-state systems). For example, a singlet $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle / \sqrt{2}$.

But thinking more about the singlet state, we seem to have found a physically inconsistent result. The entropy of the whole system is 0 because it is in a pure state, but if we can only perform measurements on one spin, then the density matrix describing those measurements has one bit of entropy. Has the physics somehow changed because we only look at one part of the system? What does it mean if a part of a system looks like a mixed state if in fact the whole system is in a pure state?

This type of question was first asked by Einstein, Podolsky, and Rosen in a famous paper in the early days of quantum mechanics. Their idea, more precisely, was to create a singlet pair of particles (there are indeed physical processes that tend to create singlets) and then spatially separate the
particles. The fact that their spins remain in the singlet indicates some type of correlation between the particles: for example, if the state of one (say, up or down along the \( z \)-axis) is known then the state of the other is known. In fact, one can make a stronger statement than this: the standard interpretation of measurement in quantum mechanics (the “Copenhagen interpretation”) is that the state of the two-spin system actually changes instantaneously as a result of measuring one spin. Since the two-spin system may be extended over a long region of space, Einstein worried that this instantaneous action at a distance must violate the basic ideas of relativity.

A partial resolution to this puzzle can be obtained by asking if any measurement on subsystem \( \mathcal{A} \) can tell whether a measurement of \( S_z \) has taken place on subsystem \( \mathcal{B} \). The density matrix of the whole system changes as a result of the measurement: it goes from the singlet (a pure state) to the mixed state with \( p = 1/2 \) to be \( | \uparrow \downarrow \rangle \) and \( p = 1/2 \) to be \( | \downarrow \uparrow \rangle \). However, the reduced density matrix for subsystem \( \mathcal{A} \) is (12), \textit{both before and after the measurement}. Hence density matrices give us a quick way to see that no observer of only \( \mathcal{A} \) can tell whether \( \mathcal{B} \) has been measured, and that whatever change in the state has occurred as a result of the measurement of \( \mathcal{B} \) is not detectable locally at \( \mathcal{A} \).