Density matrix theory

Before we can start having fun with more complicated problems, we need to develop some more sophisticated tools for dealing with thermal states. Recall that the expectation value of an observable A in equilibrium was given by

$$\langle A \rangle = \sum_n \langle n | A | n \rangle P_n \tag{1}$$

where $P_n = e^{-\beta E_n}/Z$. This is a weird kind of average because it mixes quantum expectation values, $\langle n|A|n\rangle$, with classical expectation values $\sum_n (\dots) P_n$. Moreover, as we discussed in the previous lecture, it is in general not possible to find a ket $|\psi\rangle$ that can be associated to a Gibbs state.

This motivates the introduction of a new object, called the density matrix, which generalizes the notion of ket. The density matrix of the Gibbs state is defined as

$$\boxed{\rho = \sum_n \frac{e^{-\beta E_n}}{Z} |n\rangle\langle n|} \tag{2}$$

It is therefore a sum of projection operators $|n\rangle\langle n|$, with statistical weights given by the probabilities P_n. Before I explain why it makes sense to define an object such as this, let us first see how to rewrite the average (1) in terms of ρ.

This is done using the concept of a <u>trace</u>

$$\mathrm{tr}(M) := \sum_{m} \langle m|M|m\rangle \qquad (3)$$

Some quick properties of the trace that you should definitely know

- Independent of basis choice: $\sum_{m} \langle m|M|m\rangle = \sum_{i} \langle i|M|i\rangle$
- Sum of eigenvalues: $\mathrm{tr}(M)$ = sum of eigs of M. (4)
- Cyclic: $\mathrm{tr}(AB) = \mathrm{tr}(BA)$
  $\mathrm{tr}(ABC) = \mathrm{tr}(CAB) \neq \mathrm{tr}(ACB)$ (5)
- $\mathrm{tr}(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$ (6)

Using (6) in particular, we see that (1) may be written as

$$\boxed{\langle A\rangle = \mathrm{tr}(A\rho)} \qquad (7)$$

or $\mathrm{tr}(\rho A)$ since the trace is cyclic. This equation represents the generalization of expectation values to density matrices, with the Gibbs state (2) being just one particular case.

Meaning of the density matrix

Density matrices are designed so as to combine quantum states with ignorance. If the quantum state of a system is $|\psi\rangle$ then its density matrix is defined as

$$\rho = |\psi\rangle\langle\psi| \tag{8}$$

which is called a pure state. In this case Eq (7) becomes

$$\langle A\rangle = \mathrm{tr}(A|\psi\rangle\langle\psi|) = \langle\psi|A|\psi\rangle \tag{9}$$

which is just the familiar quantum mechanical expression.

However, it could be that we don't know exactly what the state of the system is. That is, we have some degree of ignorance about it. For instance maybe the state is $|\psi_1\rangle$ with probability q_1 or maybe it is $|\psi_2\rangle$ with probability $q_2 = 1 - q_1$. The corresponding density matrix would then be

$$\rho = q_1|\psi_1\rangle\langle\psi_1| + q_2|\psi_2\rangle\langle\psi_2| \tag{10}$$

which is what we call a mixed state. Then (7) would become

$$\langle A\rangle = q_1\langle\psi_1|A|\psi_1\rangle + q_2\langle\psi_2|A|\psi_2\rangle \tag{11}$$

which, just like the Gibbs state, is a mixture of quantum averages $\langle\psi|A|\psi\rangle$ with classical averages $\sum_i (\cdots) p_i$.

In this way, the density matrix offers a generalization to the concept of ket, by treating together quantum features and classical probability theory.

For instance, suppose we have a qubit which is prepared 99% of the time in the north pole of the Bloch sphere, $|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. However, 1% of the time the machine preparating it commits an error and spits out a state

$$|\psi_2\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix}$$

where $\theta = 5°$ (just to have some concrete numbers). The state of the system in this case will not be a pure state, but rather a mixed state of the form

$$\rho = q_1 |\psi_1\rangle\langle\psi_1| + q_2 |\psi_2\rangle\langle\psi_2| \tag{12}$$

where $q_1 = 0.99$ and $q_2 = 0.01$. We can also write it more explicitly:

$$|\psi_1\rangle\langle\psi_1| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \quad 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$|\psi_2\rangle\langle\psi_2| = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix} \left(\cos\frac{\theta}{2} \quad \sin\frac{\theta}{2}\right) = \begin{pmatrix} \cos^2\theta/2 & 2\sin\theta \\ 2\sin\theta & \sin^2\theta/2 \end{pmatrix}$$

Thus

$$\rho = \begin{pmatrix} q_1 + q_2 \cos^2\theta/2 & 2q_2 \sin\theta \\ 2q_2 \sin\theta & q_2 \sin^2\theta/2 \end{pmatrix} \tag{13}$$

I know it looks ugly, but that's what it is

Of course, in (10) I considered only two possibilities. But the definition is more general. Given any set of states $|\psi_i\rangle$ and a corresponding set of probabilities q_i, the density matrix will be given by

$$\boxed{\begin{gathered} \rho = \sum_i q_i |\psi_i\rangle\langle\psi_i| \\ q_i \in [0,1], \quad \sum_i q_i = 1. \end{gathered}} \tag{14}$$

Now suppose the machine is actually quite crappy so that half of the time it prepares the state $|z_+\rangle = |\sigma = +1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and half of the time the state $|z_-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Then (12) becomes

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad (15)$$

This is called the *maximally mixed state*: it cannot get more ignorant than this. It means we know absolutely nothing about the system.

Instead, suppose now that the machine prepares with 50/50 probability the states

$$|x_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |x_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad (16)$$

then

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad (17)$$

Thus, in this case we get the same state as (15), even though we began in drastically different situations. This is called the *ambiguity of mixtures*; when we mix stuff we loose information about what we began with in the first place.

Here are some <u>general</u> <u>properties</u> of <u>the density</u> <u>matrix</u>, which can be derived solely from (14):

1) $$\rho^{\dagger} = \rho \tag{18}$$

2) $$\boxed{\operatorname{tr}(\rho) = 1} \qquad \text{Normalization of the quantum state} \tag{19}$$

check: $\operatorname{tr}(\rho) = \sum_i q_i \operatorname{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i q_i \underbrace{\langle\psi_i|\psi_i\rangle}_{1} = 1.$

3) Since ρ is Hermitian it can be diagonalized as

$$\boxed{\rho = \sum_k p_k \, |k\rangle\langle k|} \tag{20}$$

for some basis $|k\rangle$. From $\operatorname{tr}(\rho) = 1$ we see that

$$\sum_k p_k = 1 \tag{21}$$

4) For any state $|\phi\rangle$,

$$\langle\phi|\rho|\phi\rangle = \sum_i q_i \, |\langle\phi|\psi_i\rangle|^2 \geq 0 \tag{22}$$

= Prob. of finding state $|\phi\rangle$ given the system is at ρ.

5) ρ is positive semi-definite: all $p_k \geq 0$.

Proof: put $|\phi\rangle = |k\rangle$ in (22).

combined with (21) this gives

$$\boxed{p_k = \text{eigs}(\rho): \qquad p_k \in [0,1], \quad \sum_k p_k = 1} \tag{23}$$

Thus, the eigenvalues of ρ behave like probabilities

We define the <u>purity</u> of the state ρ as

$$\boxed{\text{Purity} = \operatorname{tr}(\rho^2) \leq 1} \tag{24}$$

The reason why the purity is ≤ 1 is because the eigenvalues of ρ^2 are p_k^2. Since the trace is the sum of the eigenvalues, we get $\text{Purity} = \sum_k p_k^2 \leq 1$ due to (23).

The purity will be 1 if and only if one of the p_k is 1 and the others are zero. Thus

$$\text{Purity} = 1 \quad \text{if} \quad \rho = |k_0\rangle\langle k_0| \quad \text{for some } k_0 \tag{25}$$

which is precisely a pure state, like (8). Thus, the smaller the purity the more mixed is the state.

Bloch's sphere for mixed states

Let us consider once again the case of a qubit. The density matrix will be 2×2 so we may parametrize it as

$$\rho = \begin{pmatrix} p & c \\ c^* & 1-p \end{pmatrix} \tag{26}$$

where $p \in [0,1]$ is the population and c is the coherence. To further clarify the meaning of these parameters, it is convenient to note that

$$\begin{aligned} \langle \sigma_z \rangle &= \mathrm{tr}(\sigma_z \rho) = 2p - 1 \\ \langle \sigma_x \rangle &= \mathrm{tr}(\sigma_x \rho) = c + c^* \\ \langle \sigma_y \rangle &= \mathrm{tr}(\sigma_y \rho) = i(c - c^*) \end{aligned} \tag{27}$$

Thus, if we define

$$s_\alpha = \langle \sigma_\alpha \rangle \tag{28}$$

then we may also parametrize ρ as

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + s_z & s_x - i s_y \\ s_x + i s_y & 1 - s_z \end{pmatrix} = \frac{1}{2}(1 + \vec{s} \cdot \vec{\sigma}) \tag{29}$$

I will leave for you as an exercise to compute the purity (24) of this state. It reads

$$\mathrm{tr}(\rho^2) = \frac{1 + s_x^2 + s_y^2 + s_z^2}{2} = \frac{1 + s^2}{2} \tag{30}$$

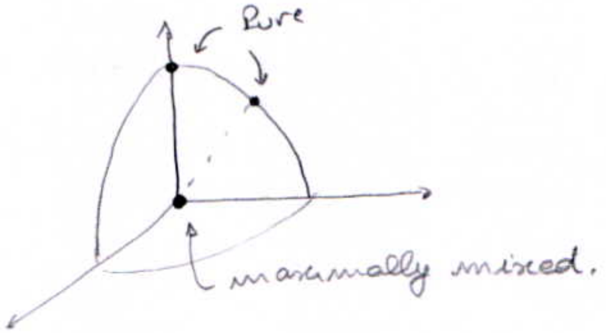
For instance, the maximally mixed state (15) has the smallest possible purity

$$\mathrm{tr}(\rho^2) = \frac{1}{2}, \quad s = 0 \tag{31}$$

This offers us an interesting interpretation: we previously saw that pure states live on the surface of the unit sphere. Now we can say that mixed states live <u>inside</u> <u>Bloch's sphere</u>. Moreover, the radius of the Bloch sphere quantifies the purity

$$s^2 = s_x^2 + s_y^2 + s_z^2 = \begin{cases} 0 & \text{maximally mixed} \\ 1 & \text{pure state} \end{cases} \tag{32}$$

Graphically this looks like this



Summary : density matrix for the Gibbs state

Now that we know better about the general features of the density matrix, let us go back to the Gibbs state (2). We can write the Hamiltonian as

$$H = \sum_m E_m |m\rangle\langle m| \tag{33}$$

Consequently

$$e^{-\beta H} = \sum_m e^{-\beta E_m} |m\rangle\langle m| \tag{34}$$

This allows us to write the partition function and the Gibbs DM more compactly as

$$\boxed{\rho = \frac{e^{-\beta H}}{Z}, \qquad Z = \mathrm{tr}(e^{-\beta H})} \tag{35}$$

This is a more sophisticated way of expressing the Gibbs state and is cool because it is basis independent. But of course, this is absolutely equivalent to what we've been doing before.

Tensor product

Now let's pause with density matrices for a second and let's review how to model quantum systems composed of multiple parts. For concreteness, suppose we have two qubits, A and B. To each qubit we associate a set of Pauli operators $\sigma_x^A, \sigma_y^A, \sigma_z^A$ and $\sigma_x^B, \sigma_y^B, \sigma_z^B$. In order for physics to make sense, we then require that taken as two separate sets, the A operators and B operators behave just like the usual Pauli operators. But, when combined, we postulate that they should commute. Thus

$$[\sigma_x^A, \sigma_y^A] = 2i\,\sigma_z^A \tag{36}$$

but

$$[\sigma_x^A, \sigma_y^B] = 0 \tag{37}$$

and so on. This kind of structure is to be taken as a postulate of quantum mechanics.

The mathematical structure behind this is called the tensor product (or Kronecker product). The tensor product of two operators A and B is written as $A \otimes B$ and is defined so as to satisfy the following property

$$\boxed{(A \otimes B)(C \otimes D) = AC \otimes BD} \tag{38}$$

That is, $\otimes$ separates two universes. Stuff to the left of $\otimes$ only talks to stuff on the left and stuff on the right of $\otimes$ only talks to stuff on the right. It makes sense (at least in my head!) as it separates systems A and B.

Thus, going back to the Pauli matrices, we actually have

$$\boxed{\begin{aligned} \sigma_i^A &= \sigma_i \otimes I_2 \\ \sigma_i^B &= I_2 \otimes \sigma_i \end{aligned}} \qquad i \in \{x, y, z\} \tag{39}$$

where I_2 is the 2×2 identity matrix. Thus, when we write it like this, Eqs (36) and (37) become true by construction.

The same kind of separation is also true for states. Let $|i\rangle_A$ be a basis for system A and $|j\rangle_B$ for system B. Then a basis for the composite system AB will be

$$\boxed{|i,j\rangle \equiv |i\rangle_A \otimes |j\rangle_B \equiv |i\rangle_A |j\rangle_B} \tag{40}$$

I write this in multiple notations because depending on the calculation one notation is better than the other. Thus, the most general pure state of AB may be written as

$$|\psi\rangle = \sum_{ij} \psi_{ij} \, |i\rangle \otimes |j\rangle \tag{41}$$

For instance, in the case of qubits we could use as basis the states $|\sigma_A\rangle$ and $|\sigma_B\rangle$, where $\sigma_{A(B)} = \pm 1$. Then a basis for two qubits would be $|\sigma_A, \sigma_B\rangle$ and a general state would be written as

$$|\psi\rangle = \sum_{\sigma_A, \sigma_B} \psi_{\sigma_A, \sigma_B} |\sigma_A, \sigma_B\rangle = \psi_{++} |++\rangle + \psi_{-+} |-+\rangle + \psi_{+-} |-+\rangle + \psi_{--} |--\rangle \tag{42}$$

The basis $|\sigma_A, \sigma_B\rangle$ is simultaneously an eigenbasis of σ_z^A and σ_z^B

$$\sigma_z^A |\sigma_A, \sigma_B\rangle = \sigma_A |\sigma_A, \sigma_B\rangle \qquad \sigma_z^B |\sigma_A, \sigma_B\rangle = \sigma_B |\sigma_A, \sigma_B\rangle \tag{43}$$

The ordering I used in Eq (42) is called lexicographic order. You first loop over the last system and then over the first, so the basis is taken as

$$|++\rangle, \; |+-\rangle, \; |-+\rangle, \; |--\rangle \tag{44}$$

This kind of ordering is quite standard. And an advantage of it is that it provides an easy way of writing $A \otimes B$ as a big matrix: You simply decompose it in a Block structure as

$$A \otimes B = \begin{pmatrix} a_{11} B & a_{12} B & \dots & a_{1N} B \\ a_{21} B & a_{22} B & \dots & a_{2N} B \\ \vdots & \vdots & \ddots & \\ a_{N1} B & a_{N2} B & & a_{NN} B \end{pmatrix} \tag{45}$$

and then expand out B.

For instance

$$\sigma_x \otimes I_2 = \begin{pmatrix} 0\, I_2 & 1\, I_2 \\ 1\, I_2 & 0\, I_2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{46}$$

and

$$I_2 \otimes \sigma_x = \begin{pmatrix} 1\, \sigma_x & 0\, \sigma_x \\ 0\, \sigma_x & 1\, \sigma_x \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{47}$$

Any numerical library has functions for quickly implementing this type of operation.

Of course, everything I said is readily generalized to N systems. Then (taking qubits as an example) we would have something like

$$\begin{aligned}\sigma_x^1 &= \sigma_x \otimes I_2 \otimes I_2 \otimes \dots \otimes I_2 \\ \sigma_x^2 &= I_2 \otimes \sigma_x \otimes I_2 \otimes \dots \otimes I_2 \\ \sigma_x^3 &= I_2 \otimes I_2 \otimes \sigma_x \otimes \dots \otimes I_2 \\ &\vdots\end{aligned} \tag{48}$$

and general basis elements

$$|\sigma_1 \dots \sigma_N\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \dots \otimes |\sigma_N\rangle \tag{49}$$

Entanglement and mixed states

Let us focus on qubits and I'll write the computational basis as $|0\rangle$ and $|1\rangle$ for now. Consider then the state

$$|\psi\rangle = \frac{1}{2}\left(|00\rangle + |01\rangle + |10\rangle + |11\rangle\right) \tag{50}$$

this state looks rather complicated. However, with some thought we can see that it may be written as (please check!)

$$|\psi\rangle = \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \otimes \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \tag{51}$$

Thus, this state corresponds to the two qubits in well defined states. they are both in the + eigenstate of σ_x

$$|x+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \tag{52}$$

$$\sigma_x |x+\rangle = |x+\rangle$$

Instead of (50), consider now the state

$$|\psi\rangle = \frac{1}{2}\left(|00\rangle + |01\rangle + |10\rangle - |11\rangle\right) \tag{53}$$

This seems at first quite analogous to (50). However, it turns out, it is impossible to write this as a product state, like (51). Whenever a state cannot be written as a product state, we say it is entangled.

In fact, an easy way to see that (53) is fundamentally different is to note that

$$\langle \psi | \sigma_x^1 | \psi \rangle = \langle \psi | \sigma_x^2 | \psi \rangle = 0 \tag{54}$$

which is in huge contrast to (52). In fact, quite remarkably, for the state (53) it follows that we also have

$$\begin{aligned} \langle \psi | \sigma_y^1 | \psi \rangle &= \langle \psi | \sigma_y^2 | \psi \rangle = 0 \\ \langle \psi | \sigma_z^1 | \psi \rangle &= \langle \psi | \sigma_z^2 | \psi \rangle = 0 \end{aligned} \tag{55}$$

Now let's see how entangled states look like, if we shift our focus to one of the subsystems only. For simplicity let us suppose that our state has the form

$$|\psi\rangle = \sum_i c_i |i, i\rangle \qquad (56)$$

where the c_i are coefficients. Since $\langle\psi|\psi\rangle = 1$ we must have

$$\sum_i |c_i|^2 = 1 \qquad (57)$$

Now let's compute the expectation value of some observable A that lives only on subsystem 1. It is given by

$$\langle A_1\rangle = \langle\psi|(A\otimes I)|\psi\rangle = \sum_{ij} c_i^* c_j \langle i i|(A\otimes I)|j j\rangle \qquad (58)$$

This type of multiplication is something I really want you to know how to do. All you need to remember is the separate universes property (38):

$$\langle i,i|A\otimes I|j,j\rangle = \langle i|A|j\rangle \underbrace{\langle i|I|j\rangle}_{\delta_{ij}} = \langle i|A|i\rangle\,\delta_{ij}$$

Thus we get

$$\langle A_1\rangle = \sum_i |c_i|^2 \langle i|A|i\rangle \qquad (59)$$

We now ask whether it is possible to associate a state with system 1 only. But Eq (59) should remind you of Eq (1): it is a mixture of $\langle i|A|i\rangle$ with probabilities $|c_i|^2$. Thus, the state of 1 will actually be a mixed state described by a density matrix

$$\rho_1 = \sum_i |c_i|^2 |i\rangle\langle i| \qquad (60)$$

This is a very very very very very important result

The state (56) is in general entangled. It will only be a product state when $c_j = 1$ and all other $c_i = 0$. In this case (60) will be a pure state $|j\rangle\langle j|$. Otherwise it will be mixed.

The take home message then, is that

If the global system is entangled, the reduced systems will be in a mixed state (61)

Recall that when we first defined the DM, we said it was an object that encompassed both quantum physics plus ignorance. Before we considered that this ignorance was of classical origin (a faulty machine, for instance). But now we see that ignorance may also be of quantum origin, stemming from the entanglement of a system with its surroundings.

Partial trace

We arrived at Eq (60) in a somewhat funny way, by looking at $\langle A_1 \rangle$. But now we can make this kind of operation more systematic. This is done using the idea of a partial trace. The trace is an operation which transforms operators into numbers. The partial trace does the same, but only for one part of the Hilbert space.

For instance, if ρ_{12} is a density matrix for the composite system then

$$\mathrm{tr}\,\rho_{12} = \sum_{ij} \langle i,j | \rho_{12} | i,j \rangle = 1 \tag{62}$$

In the partial trace, we sum only one of the basis sets:

$$\rho_1 = \mathrm{tr}_2\, \rho_{12} = \sum_j {}_2\langle j | \rho_{12} | j \rangle_2 \tag{63}$$

$$\rho_2 = \mathrm{tr}_1\, \rho_{12} = \sum_i {}_1\langle i | \rho_{12} | i \rangle_1 \tag{64}$$

The result is still an operator, but living on a smaller Hilbert space. Note I write $|j\rangle_2$ and $|i\rangle_1$ to clarify that these are kets acting only on specific Hilbert spaces.

Another, more intuitive way of writing the partial trace is as follows. First note that

$$\mathrm{tr}(A \otimes B) = \sum_{ij} \langle ij | A \otimes B | ij \rangle$$

$$= \sum_i \langle i | A | i \rangle \sum_j \langle j | B | j \rangle$$

Thus

$$\mathrm{tr}(A \otimes B) = \mathrm{tr}(A)\,\mathrm{tr}(B) \tag{65}$$

the partial trace will now do only part of the job

$$\boxed{\begin{aligned} \mathrm{tr}_1(A \otimes B) &= \mathrm{tr}(A)\,B \\ \mathrm{tr}_2(A \otimes B) &= A\,\mathrm{tr}(B) \end{aligned}} \tag{66}$$

As an example, consider two qubits in the state

$$|\psi\rangle = \sqrt{p}\,|00\rangle + \sqrt{1-p}\,|11\rangle \tag{67}$$

this state is pure so the global density matrix will be simply given by

$$\begin{aligned} \rho_{12} = |\psi\rangle\langle\psi| &= p\,|00\rangle\langle 00| + (1-p)\,|11\rangle\langle 11| \\ &\quad + \sqrt{p(1-p)}\,|00\rangle\langle 11| + \sqrt{p(1-p)}\,|11\rangle\langle 00| \end{aligned} \tag{68}$$

Now let's trace system 2. We have, using (66)

$$\mathrm{tr}_2\,|00\rangle\langle 00| = |0\rangle\langle 0|\,\underbrace{\mathrm{tr}(|0\rangle\langle 0|)}_{\langle 0|0\rangle = 1}$$

$$\mathrm{tr}_2\,|00\rangle\langle 11| = |0\rangle\langle 1|\,\underbrace{\mathrm{tr}(|0\rangle\langle 1|)}_{\to 0}$$

and so on. Thus

$$\rho_1 = \mathrm{tr}_2\,\rho_{12} = p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1| \tag{69}$$

$$= \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}$$

This introduces us to the real idea of purification. Suppose we have a system prepared in a Gibbs state

$$\rho = \sum_n \frac{e^{-\beta E_n}}{Z} |n\rangle\langle n| \qquad (70)$$

This is in general a mixed state, unless $T=0$. But now we can think that this mixed state is actually an entangled state between the system and the environment. There is an infinite number of environments and configurations which, from the perspective of the system, would give the state (70).

For instance, if we assume (which is a bit fake) that the environment is an identical copy of the system, then one possible dilation would be

$$|\psi\rangle = \sum_n \sqrt{\frac{e^{-\beta E_n}}{Z}}\, |n,n\rangle \qquad (71)$$

As another example, suppose that A and B are in the entangled state

$$|\psi\rangle = \sqrt{p}\,|0,1\rangle + \sqrt{1-p}\,|1,0\rangle \qquad (72)$$

then

$$\begin{aligned} \rho_A &= p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1| \\ \rho_B &= p|1\rangle\langle 1| + (1-p)|0\rangle\langle 0| \end{aligned} \qquad (73)$$

If we let p be the Fermi Dirac distribution

$$p = \frac{1}{e^{\beta\epsilon}+1}$$

then

$$1-p=\frac{1}{e^{-\beta\epsilon}+1}$$

Hence, if A is at a positive temperature, then B will be in a negative temperature. It looks like if A is the real world, then B is the upside down from Stranger Things.

van Neumann entropy

The entropy of a quantum state ρ is known as the van Neumann entropy and is defined as

$$\boxed{S(\rho) = -\,\mathrm{tr}(\rho \ln \rho)} \qquad (74)$$

This generalizes the Gibbs-Shannon entropy to density matrices. If we write the eigenstuff equation for ρ as

$$\rho|k\rangle = p_k|k\rangle \qquad (75)$$

then we can choose the basis $|k\rangle$ to take the trace in (74). This then yields

$$S(\rho) = -\sum_k p_k \ln p_k \qquad (76)$$

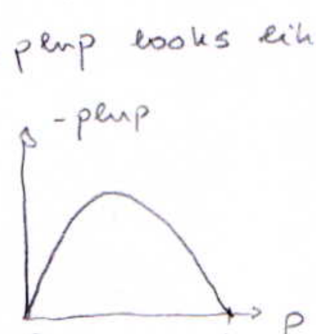
so that, written in this way, it looks formally identical to the Gibbs-Shannon entropy. However, this doesn't mean that they are actually the same, as we will see below.

The van Neumann entropy (74) is bounded as

$$\boxed{0 \leqslant S(\rho) \leqslant \ln(d)} \qquad (77)$$

where d is the dimension of the Hilbert space.

The value $S=0$ occurs for pure states. Then $p_{k'}=1$ and $p_k=0$ for $k\neq k'$. Recalling that $-p\ln p$ looks like



we then get

$$\boxed{S(\rho) = 0 \quad \text{if } \rho \text{ is a pure state}} \tag{78}$$

conversely, the limit $S = \ln(d)$ occurs for the maximally mixed state

$$\boxed{S(\rho) = \ln(d) \quad \text{if} \quad \rho = \frac{I_d}{d}} \tag{79}$$

For this reason, the entropy quantifies the <u>amount</u> of <u>information</u> we have about the state of the system. the larger the entropy, the less we know.

It is then convenient to define the <u>information</u> in ρ as

$$I(\rho) = \ln(d) - S(\rho) \tag{80}$$

then if the state is pure $(S=0)$ we have a total of $\ln(d)$ of information and if the state is maximally mixed, we have zero information.

Another extremely important quantity is the relative entropy, or Kullback - Leibler divergence,

$$\boxed{S(\rho\|\sigma) = \mathrm{tr}\left(\rho\ln\rho - \rho\ln\sigma\right) \geq 0} \tag{81}$$

where ρ and σ are two arbitrary density matrices. The relative entropy is always non-negative being zero if and only if $\rho = \sigma$. I will not demonstrate this here, but you can find the proof in Nielsen and Chuang (and also on Wikipedia). But this fact means that $S(\rho\|\sigma)$ functions as a type of distance between density matrices.

Next let $\pi = \mathrm{Id}/d$ denote the maximally mixed state. Then

$$\begin{aligned} S(\rho\|\pi) &= \mathrm{tr}(\rho\ln\rho) - \mathrm{tr}(\rho\ln\pi) \\ &= -S(\rho) - \sum_k \langle k|\rho\ln\pi|k\rangle \\ &= -S(\rho) - \sum_k p_k \ln(1/d) \\ &= -S(\rho) + \ln(d) \end{aligned}$$

Thus we see that

$$S(\rho) = \ln(d) - S(\rho\|\pi) \tag{82}$$

Consequently, the information (80) can be written as

$$\boxed{I(\rho) = S(\rho\|\pi)} \tag{83}$$

This allows for a cool interpretation: the information is the distance between the state ρ and maximally mixed state, which is the completely ignorant state. Makes sense!

Next let

$$\rho_{eq} = \frac{e^{-\beta H}}{Z} \tag{84}$$

and let us compute

$$S(\rho \| \rho_{eq}) = - S(\rho) - \mathrm{tr}(\rho \ln \rho_{eq})$$

$$= -S(\rho) - \mathrm{tr}\left\{ \rho \left[-\beta H - \ln Z \right] \right\}$$

$$= -S(\rho) + \beta\, \mathrm{tr}(H\rho) + (\ln Z)\, \underbrace{\mathrm{tr}(\rho)}_{1}$$

$$= -S(\rho) + \beta U(\rho) + \ln Z$$

where

$$U(\rho) = \mathrm{tr}(H\rho) \tag{85}$$

is the average energy in a given state ρ (not necessarily equilibrium). If we multiply by T on both sides, we then get

$$T\, S(\rho \| \rho_{eq}) = U(\rho) - TS(\rho) + T \ln Z \tag{86}$$

We now identify here two elements. The first is the equilibrium free energy

$$F_{eq} = -T \ln Z \tag{87}$$

and the second is a non-equilibrium free energy

$$F(\rho) = U(\rho) - TS(\rho) \tag{88}$$

Thus we see that by rearranging (86) we can write

$$\boxed{F(\rho) = F_{eq} + T\, S(\rho \| \rho_{eq})} \tag{89}$$

In my opinion this result is really cool. Since $S(\rho\|\rho_{eq}) \geq 0$ it implies that

$$\boxed{F(\rho) \geq F_{eq}} \tag{90}$$

Since this inequality holds for arbitrary ρ, it follows that equilibrium is the state which minimizes the free energy. Any non-equilibrium state will have a larger $F(\rho)$. It's also cool to contrast this with the information (83). We see that just like information is a distance to a maximally mixed state, free energy is a difference to an equilibrium state

Eq (90) is also the starting point for a powerful approximation method known as the Bogoliubov variational method. Do you remember the variational method in quantum mechanics? It went something like this: we a have system with Hamiltonian H and we want to know the ground-state energy E_{gs}, but we can't do it exactly because the Hamiltonian is too complicated. However, given an arbitrary state $|\psi\rangle$, it turns out that

$$E_{gs} \leq \langle\psi|H|\psi\rangle \tag{91}$$

This therefore provides us with a strategy for estimating a bound on E_{gs}. Simply choose a $|\psi\rangle$ with many free parameters and then minimize $\langle\psi|H|\psi\rangle$. The result will be an upper bound on E_{gs}. If you choose very good $|\psi\rangle$'s, you will get closer and closer to E_{gs}.

We can now do the same with thermal equilibrium and Eq (90). Suppose we are given a Hamiltonian H and we want to compute

$$F_{eq} = -T \ln Z = -T \ln \operatorname{tr} e^{-\beta H} \tag{92}$$

But that's too hard. However, from (90) we know that any ρ we choose will give a upper bound on F_{eq}. A natural choice for ρ is then another thermal state, but with a simpler Hamiltonian H_0 that we know how to deal with. That is

$$\rho = \rho_0 = \frac{e^{-\beta H_0}}{Z_0} \qquad Z_0 = \operatorname{tr} e^{-\beta H_0} \tag{93}$$

Then we will have

$$F(\rho_0) = \langle H\rangle_0 - T\,S(\rho_0) \tag{94}$$

But since ρ_0 is a thermal state

$$S(\rho_0) = \frac{\langle H_0\rangle_0 - F_0}{T} \tag{95}$$

where

$$F_0 = -T \ln Z_0 \tag{96}$$

Thus

$$F(\rho_0) = \langle H \rangle_0 - \langle H_0 \rangle_0 + F_0 \tag{97}$$

Inserting this in Eq (90) we then obtain the Bogoliubov variational formula

$$\boxed{F_0 + \langle H - H_0 \rangle_0 \geqslant F_{eq}} \tag{98}$$

The method then works like this: choose an H_0 that you know how to deal with and has some free parameters. Then compute F_0, $\langle H_0 \rangle_0$ and $\langle H \rangle_0$. The latter, in particular, should not be too hard since even though H is tough, the average here is over ρ_0 and not ρ_{eq} (which you don't know). Then the quantity on the LHS of (98) will give you an upper bound on the true equilibrium free energy F_{eq}

Mutual Information

As a last topic of these notes, we discuss the van Neumann entropy for reduced density matrices. Consider a bipartite system AB with a density matrix ρ_{AB}. then let

$$\begin{aligned} \rho_A &= \mathrm{tr}_B\, \rho_{AB} \\ \rho_B &= \mathrm{tr}_A\, \rho_{AB} \end{aligned} \tag{99}$$

In general it turns out that

$$S(\rho_A) + S(\rho_B) \geqslant S(\rho_{AB}) \tag{100}$$

this is called subadditivity of the van Neumann entropy. the equality only holds when A and B are in a product state

$$\rho_{AB} = \rho_A \otimes \rho_B \tag{101}$$

Eq (100) motivates us to define the mutual information

$$\boxed{I(A:B) := S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \geqslant 0} \tag{102}$$

the mutual information quantifies the amount of correlations between A and B. this becomes more evident if we use the concept of information defined in (80). We then get

$$\boxed{I_{AB} = I_A + I_B + I(A:B)} \tag{103}$$

Thus, the total amount of information contained in AB is equal to the information locally contained in A and B, plus the mutual information $I(A:B)$. Hence $I(A:B)$ is the amount of information that is not contained locally, but requires knowledge of the full state ρ_{AB}.

One may also show that $I(A:B)$ may be written as

$$\boxed{I(A:B) = S(\rho_{AB} \| \rho_A \otimes \rho_B)} \qquad (104)$$

Hence, it is the distance between the actual state ρ_{AB} and the marginalized state $\rho_A \otimes \rho_B$. Again, makes sense!

In general $I(A:B)$ quantifies all correlations between A and B, irrespective of whether they are classical or quantum. But if $\rho_{AB} = |\psi\rangle\langle\psi|$ is a pure state then $S(\rho_{AB}) = 0$ and, it turns out $S(\rho_A) = S(\rho_B)$ (I will not prove this here but you can find it on Sec 2.9 of my quantum information notes). Then

$$I(A:B) = 2S(\rho_A) = 2S(\rho_B)$$

In this case $S(\rho_A)$ (or $S(\rho_B)$) is called the entanglement entropy: when AB is pure, the correlations are purely quantum (purely entanglement). The mutual info is then simply twice the entanglement entropy.