

Physics 342 Lecture 38

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Welcome back for more quantum, density matrix style. In the previous lecture, we had introduced mixed states as the most general state in which an ensemble of quantum particles can live. A mixed state is defined by a collection of pure states $\{|\psi_i\rangle\}_i$, which live in the Hilbert space, and probabilities $\{w_i\}_i$ for the particles to be in the i^{th} pure state. We had defined the density matrix ρ as the object that encodes all of this information, where

$$\rho = \sum_{i \text{ pure}} w_i |\psi_i\rangle\langle\psi_i|. \text{ The density matrix satisfies a}$$

number of interesting properties, including selfadjointness: $\rho = \rho^\dagger$, and its time evolution equation:

$$i\hbar \frac{\partial \rho}{\partial t} = [\hat{H}, \rho], \text{ where } \hat{H} \text{ is the Hamiltonian on the Hilbert space.}$$

Further, we had also shown that conservation of probability/unitarity is encoded in the trace of ρ : $\text{tr } \rho = \sum_{i \text{ pure}} w_i = 1$. In this lecture, we ~~are~~ are going to quantify the degree to which the system is mixed. We had first hints of this last lecture. Only for a pure state is the density matrix idempotent, or that its square is equal to itself: $\rho^2 = \rho$, for pure states. Correspondingly, as $\text{tr } \rho = 1$, for a pure state $\text{tr } \rho^2 = 1$, as well, and this property can equally define a pure state.

Now, we are always able to write the density matrix in diagonal form, where the w_i fractions occupy the diagonal entries; and 0s everywhere else:

$$\rho^{(\text{diag})} = \begin{pmatrix} w_1 & & & \\ & w_2 & & \\ & & w_3 & \\ & & & \dots \\ & & & & w_N \end{pmatrix}.$$

The trace is basis-independent, and so this diagonal form helps us analyze ρ^2 .

When diagonalized, ρ^2 is:

$$(\rho^{(\text{diag})})^2 = \begin{pmatrix} w_1^2 & & & \\ & w_2^2 & & \\ & & w_3^2 & \\ & & & \dots \\ & & & & w_N^2 \end{pmatrix} \quad \text{and so its trace is}$$

$$\text{tr } \rho^2 = \sum_{i \text{ pure}} w_i^2 = \sum_{i \text{ pure}} w_i^2 + \sum_{i < j \text{ pure}} 2w_i w_j - \sum_{i < j \text{ pure}} 2w_i w_j$$

$$= \left(\sum_{i \text{ pure}} w_i \right)^2 - \sum_{i < j \text{ pure}} 2w_i w_j = 1 - \sum_{i < j \text{ pure}} 2w_i w_j.$$

In these manipulations, we just added and subtracted a quantity that enabled us to complete the square. This demonstrates that $\text{tr } \rho^2 \leq 1 = \text{tr } \rho$, as all the w_i fractions are non-negative. Thus, a single number that quantifies the degree to which an ensemble is not in a pure state can be defined to be the difference of the trace of ρ versus ρ^2 . Let's call this difference $S^{(1)}$:

$S^{(1)} \equiv \text{tr}(\rho - \rho^2)$. By the calculation above, this quantity

is non-negative, $S^{(1)} \geq 0$, and is only 0 if the system is in a pure state.

Remember that if the system is in a pure state, every one

of the quantum particles is in the same state $| \psi_i \rangle$. If the states are represented by spins, then we would say that the system is polarized. Another way to say this is that if your system is in a pure state, then you know exactly what state each individual particle occupies. If the system is not in a pure state then ~~you~~ there exists a non-zero uncertainty on the state an individual particle occupies. Thus, $S^{(1)}$ is a measure of your knowledge of the states of individual particles, given information about the ensemble. If $S^{(1)} = 0$, then information about the ensemble is sufficient to have complete, perfect knowledge of individual particle states, while if $S^{(1)} > 0$, you only have incomplete knowledge of individual particle states.

Nevertheless, $S^{(1)}$ is just one possible measure for this information. We can define a one-parameter family of measures $S^{(\alpha)}$, where

$$S^{(\alpha)} = \frac{\text{tr}(\rho^{\alpha+1})}{\alpha}, \text{ where } \alpha \text{ is a}$$

positive real number. $S^{(\alpha)}$ satisfies the same properties that $S^{(1)}$ does: $S^{(\alpha)}$ is 0 if and only if the system is in a pure state, and $S^{(\alpha)} > 0$ otherwise. This quantity is called the Rényi entropy with parameter α . Some values of α are particularly interesting. We already discussed $\alpha=1$, which exploits the idempotency of the density matrix for a pure state. As $\alpha \rightarrow \infty$, the Rényi entropy is either 0 or 1:

$$\lim_{\alpha \rightarrow \infty} \alpha S^{(\alpha)} = \lim_{\alpha \rightarrow \infty} \text{tr}(\rho^{\alpha+1}) = \begin{cases} 0, & \text{pure state} \\ 1, & \text{else,} \end{cases}$$

As the trace of $\rho^{\alpha+1}$, $\text{tr} \rho^{\alpha+1} = \sum_i w_i^{\alpha+1} \rightarrow 0$, as $\alpha \rightarrow \infty$ if any two w_i are non-zero.

However, the most interesting and important value of α is as $\alpha \rightarrow 0$. Note that

$$\begin{aligned} \frac{\rho - \rho^{\alpha+1}}{\alpha} &= \rho \frac{1 - \rho^\alpha}{\alpha} = \rho \frac{1 - e^{\alpha \ln \rho}}{\alpha} = \rho \frac{1 - 1 - \alpha \ln \rho - \dots}{\alpha} \\ &= -\rho \ln \rho, \text{ as } \alpha \rightarrow 0. \end{aligned}$$

The $\alpha \rightarrow 0$ entropy is called the von Neumann entropy and is defined to be:

$$S_{\text{VN}} \equiv -\text{tr}(\rho \ln \rho).$$

If the $\ln \rho$ scares you, don't fret: we can always work with ρ in diagonal form, or use the Taylor expansion of logarithm:

$$\ln \rho = \ln(\mathbb{1} - (\mathbb{1} - \rho)) = -(\mathbb{1} - \rho) - \frac{(\mathbb{1} - \rho)^2}{2} - \dots$$

This von Neumann entropy is non-negative by construction and only vanishes for a pure state in which $\rho = 1$, so $\ln \rho = 0$. A completely random state is a density matrix for ~~which~~ which all diagonal entries are equal; that is, for a system in which every particle occupies a distinct pure state. For such a system, your knowledge about the ensemble provides the least possible information about each particle's state, and so S_{VN} should be maximized. For a system of N particles, the completely random density matrix (when diagonalized) takes the form:

$$\rho_{\text{random}} = \begin{pmatrix} \frac{1}{N} & & & 0 \\ & \frac{1}{N} & & \\ & & \frac{1}{N} & \vdots \\ 0 & & & \frac{1}{N} \end{pmatrix}$$

and so the von Neumann entropy of such a state would be:

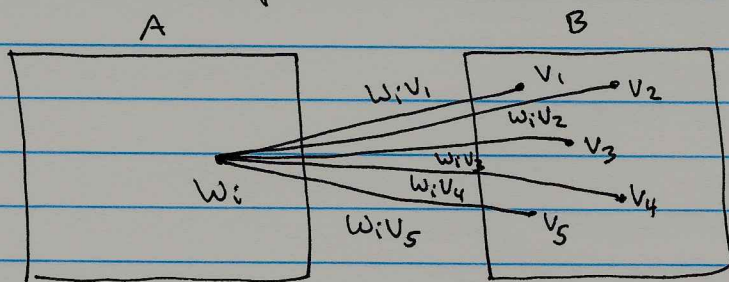
$$S_{vN} = \sum_{i=1}^N \frac{1}{N} \ln \frac{1}{N} = N \left(\frac{1}{N} \ln N \right) = \ln N.$$

Thus, in general $0 \leq S_{vN} \leq \ln N$, for an ensemble of N particles.

What makes the von Neumann entropy particularly nice and why it is the quantum mechanical entropy is due to its properties when two or more ensembles are combined. Consider two quantum ensembles, A and B , with density matrices ρ_A and ρ_B , respectively. If A and B are initially independent, but then combined to form a larger ensemble $A \oplus B$, the resulting density matrix is just the product of ρ_A and ρ_B :

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tensor

$\rho_{A \oplus B} = \rho_A \otimes \rho_B$. This can be proven easily when ρ_A and ρ_B are written in diagonal form. The tensor product means that each entry in ρ_A is multiplied by the entire matrix ρ_B . The way to interpret this is the following. Given a state of system A with probability w_i , the state of B can be anything, by their assumed independence. We can draw a picture to illustrate this:



In this figure, we have represented the ensembles as the boxes, and individual pure states by dots. Given the pure state ~~state~~ i with probability w_i in A , the probabilities for i in A and state j in B is just the product of the individual

probabilities: $P(i+j) = w_i v_j$, by the assumed independence. Now, the total probability to just be in state i in A is still w_i , which we can find by summing over the probabilities to be in any state of B :

$$P(i \text{ in } A) = \sum_{j \in B} P(i+j) = \sum_{j \in B} w_i v_j = w_i \sum_{j \in B} v_j = w_i,$$

as we have assumed that $\text{tr } \rho_A = \text{tr } \rho_B = 1$.

With this observation, we can then calculate the total entropy of the combined system:

$$\begin{aligned} S_{\text{VN}}^{A \otimes B} &= \text{tr}(\rho_A \otimes \rho_B \ln \rho_A \otimes \rho_B) = \text{tr}[\rho_A \otimes \rho_B \ln \rho_A + \rho_A \otimes \rho_B \ln \rho_B] \\ &= \text{tr}(\rho_A \ln \rho_A) + \text{tr}(\rho_B \ln \rho_B) = S_{\text{VN}}^A + S_{\text{VN}}^B. \end{aligned}$$

By the manipulations above, the logarithm of a tensor product still expands out like you are familiar with for the logarithm. That is the von Neumann entropy is additive for independent systems. This also demonstrates that you can never gain information by adding a new, independent system: Because $S_{\text{VN}} \geq 0$, we have

$$S_{\text{VN}}^{A \otimes B} \geq \max(S_{\text{VN}}^A, S_{\text{VN}}^B).$$

Many other additivity properties of the von Neumann entropy can also be shown to hold, which is not the case for the general Rényi entropies.

It's also interesting to ask about the time derivative of the entropy. To evaluate this, we will work with the Rényi entropy

As it is a bit easier to work with, but the $\alpha \rightarrow 0$ limit can be taken to find the time derivative of the von Neumann entropy. The time derivative is:

$$\frac{dS^{(\alpha)}}{dt} = \frac{d}{dt} \frac{\text{tr}(\rho - \rho^{\alpha+1})}{\alpha} = -\frac{1}{\alpha} \text{tr} \frac{d\rho^{\alpha+1}}{dt} = -\frac{\alpha+1}{\alpha} \text{tr} \left(\rho^{\alpha} \frac{1}{i\hbar} [\hat{H}, \rho] \right),$$

where we used the fact that $\text{tr} \rho = 1$ and the chain rule for differentiation. We can further massage the trace

as:

$$\frac{dS^{(\alpha)}}{dt} = -\frac{\alpha+1}{\alpha(i\hbar)} \text{tr} \left[\rho^{\alpha} \hat{H} \rho - \rho^{\alpha} \rho \hat{H} \right],$$

now, we can use the cyclicity of the trace:

$$\text{tr}(ABC) = \text{tr}(CAB). \text{ This follows from just writing}$$

the trace as a sum over explicit matrix elements:

$$\text{tr}(ABC) = \sum_{i,j,k} A_{ij} B_{jk} C_{ki} = \sum_{i,j,k} C_{ki} A_{ij} B_{jk} = \text{tr}(CAB).$$

Thus, $\text{tr}(\rho^{\alpha} \hat{H} \rho) = \text{tr}(\rho^{\alpha+1} \hat{H})$, and so

$$\frac{dS^{(\alpha)}}{dt} = -\frac{\alpha+1}{\alpha(i\hbar)} \text{tr} \left[\rho^{\alpha+1} \hat{H} - \rho^{\alpha+1} \hat{H} \right] = 0, \text{ or, the}$$

entropy is constant in time. Now you might be familiar with the second law of thermodynamics which states that the entropy of a closed system can never decrease. This, at least, is not inconsistent with that, but demonstrating that entropy can increase requires significantly more sophistication and analysis of mixed states.

We can demonstrate a related property: that a pure state

can never become a mixed state, assuming unitary time evolution. In terms of the density matrix at time $t=0$, $\rho(0)$, the density matrix at time t is just:

$$\begin{aligned} \rho(t) &= \sum_{i \text{ pure}} w_i |\psi_i(t)\rangle \langle \psi_i(t)| = \sum_{i \text{ pure}} w_i e^{-\frac{i\hat{H}t}{\hbar}} |\psi_i(0)\rangle \langle \psi_i(0)| e^{\frac{i\hat{H}t}{\hbar}} \\ &= e^{-\frac{i\hat{H}t}{\hbar}} \rho(0) e^{\frac{i\hat{H}t}{\hbar}}, \text{ assuming that the pure states} \end{aligned}$$

evolve according to the Schrödinger equation. Now, let's calculate $\rho(t)^2$: if this is $\rho(t)$, then the system is in a pure state at time t :

$$\begin{aligned} \rho(t)^2 &= e^{-\frac{i\hat{H}t}{\hbar}} \rho(0) e^{\frac{i\hat{H}t}{\hbar}} e^{-\frac{i\hat{H}t}{\hbar}} \rho(0) e^{\frac{i\hat{H}t}{\hbar}} \\ &= e^{-\frac{i\hat{H}t}{\hbar}} \rho(0)^2 e^{\frac{i\hat{H}t}{\hbar}}. \end{aligned}$$

If the system is initially in a pure state at $t=0$, then $\rho(0)^2 = \rho(0)$, and so we further find:

$$\rho(t)^2 = e^{-\frac{i\hat{H}t}{\hbar}} \rho(0)^2 e^{\frac{i\hat{H}t}{\hbar}} = e^{-\frac{i\hat{H}t}{\hbar}} \rho(0) e^{\frac{i\hat{H}t}{\hbar}} = \rho(t),$$

and thus pure states always evolve into pure states.

We'll play around with this formalism a bit more in the final lecture, as well as see some examples.