

Lecture 8: Thermality

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Now that we've formally introduced resource theories and covered the QRTs of non-uniformity and entanglement it's time to move on to the main QRT of this course: the resource theory of athermality. Before we introduce the resource theory proper and its free operations the next lecture, today we will set the scene by examining the free states: thermal states. In statistical mechanics we can derive the form of these states – the Gibbs distribution – by introducing an appropriate statistical ensemble such as the canonical ensemble. In a similar fashion, the maximum entropy principle tells us to assign the state of maximal information entropy to the system, arriving at the same distribution. In this lecture we introduce an alternative way of deriving the thermal distribution. As a starting point we find a notion of equilibrium that applies to single, finite-dimensional quantum systems. It is motivated by the argument that if a system is locally in equilibrium no unitary perturbation of its state should be able to further reduce its energy. At the individual system level this form of equilibrium is called *passivity* and the corresponding equilibrium states are accordingly called *passive states*. In the next step we can require that when we combine many identical, non-interacting passive states, they should still be in equilibrium, with respect to global unitary state changes. We will show that thermal states are the only ones for which this holds in the many-partite limit.

Equilibrium states in thermodynamics are characterised by the Gibbs distribution. Consider a finite-dimensional Hilbert space \mathcal{H} , a time-independent Hamiltonian H and the inverse temperature $\beta = (k_B T)^{-1}$. The corresponding thermal state is then given by:

$$\gamma_\beta := \frac{1}{Z} e^{-\beta H}, \quad (1)$$

with the partition sum $Z = \text{tr}[\exp(-\beta H)]$.

I Passivity

We want to establish a notion of equilibrium that applies at the level of small quantum systems characterised by a finite-dimensional Hilbert space \mathcal{H} and a time-independent Hamiltonian H . Such a quantum system is in equilibrium if it is in a state whose energy cannot be lowered by a cyclic perturbation of the system. Here, cyclicity means that the perturbation only affects the system during a certain time interval before and after which only the reference Hamiltonian H governs the energy of the system. Such a cyclic unitary interaction with the system should not be able to extract energy from the system (i.e., lower the energy of the system).

Cyclic unitary processes

Starting at time $t = 0$, the system is unitarily driven by some Hamiltonian

$$K(t) = H + V(t) \quad (2)$$

for an evolution time T with the condition that $V(t) = 0$ for $t < 0$ and $t > T$.



Due to the von Neumann equation,

$$i \frac{d\rho(t)}{dt} = [K(t), \rho(t)], \quad (3)$$

any such driving gives rise to a unitary evolution operator $U(t)$ and we have

$$\rho(t) = U(t)\rho(0)U^\dagger(t). \quad (4)$$

The (average) energy change of such a process $\rho(0) \rightarrow \rho' := \rho(T)$ is given by

$$\Delta E = \text{tr}[\rho' H] - \text{tr}[\rho H] \quad (5)$$

We call a state *passive* if this energy difference cannot be made negative for any perturbation $K(t)$ and hence any unitary interaction $U \equiv U(T)$. From this requirement we can obtain clear criteria under which a state is passive with respect to the reference Hamiltonian H .

Passive states

Given a state ρ and a reference Hamiltonian H :

$$H := \sum \epsilon_i |e_i\rangle\langle e_i|, \text{ with } \epsilon_{i+1} \geq \epsilon_i \forall i, \quad (6)$$

ρ is passive with respect to H if and only if (1) ρ and H are diagonal in the same basis and (2) ρ contains no population inversion:

- 1) $[\rho, H] = 0$, and
- 2) $\epsilon_j < \epsilon_k \Rightarrow r_j \geq r_k$, with $r_j := \langle e_j | \rho | e_j \rangle$.

In other words, for any Hamiltonian H as above, passive states are exactly those states which can be spectrally decomposed as

$$\pi = \sum r_i |e_i\rangle\langle e_i|, \text{ with } r_{i+1} \leq r_i \forall i. \quad (7)$$

Any state that is not passive is called active.

Conditions (1) and (2) can be proven with some standard matrix calculus. We do not reproduce the proof here but note that both conditions are individually rather intuitive.

Activation, N-passivity, and complete passivity

When combining two or more identical passive states $\pi^{(k)}$ (each pertaining to a Hilbert space labelled by k), the resulting multi-partite state $\bigotimes_k \pi^{(k)}$ need not be passive. This process of system combination is hence called *activation*. **Convince yourself that a combined state $\bigotimes_k \pi^{(k)}$ resulting from activation always commutes with the combined Hamiltonian $\sum_k H^{(k)}$ and thus still fulfils passivity criterion (1) automatically.** Activation thus arises due to violation of the second condition when identical systems are combined. Such a violation is called population inversion and the following example demonstrates how it can occur.

Example: Activation

Consider the passive qutrit state

$$\pi = \frac{1}{2} (|0\rangle\langle 0| + |2\rangle\langle 2|), \quad (8)$$

where $\{|0\rangle, |2\rangle, |3\rangle\}$ is an orthonormal basis, and the following Hamiltonian:

$$H = 2|2\rangle\langle 2| + 3|3\rangle\langle 3| \quad (9)$$

For the combined state $\pi \otimes \pi$ we have

$$\pi \otimes \pi = \frac{1}{4} (|0,0\rangle\langle 0,0| + |0,2\rangle\langle 0,2| + |2,0\rangle\langle 2,0| + |2,2\rangle\langle 2,2|) \quad (10)$$

which is active with respect to the combined Hamiltonian $H_{tot} = H \otimes \mathbf{I} + \mathbf{I} \otimes H$.

To see this note that the population of the energy eigenstate $|2,2\rangle$ exceeds that of the unoccupied state $|0,3\rangle$ even though the energy of the former is larger than that of the latter. Specifically, labelling the eigenvalues of H_{tot} as $E_{n,m}$ and the corresponding populations as $p_{n,m}$, we have

$$p_{2,2} = \frac{1}{4} > 0 = p_{0,3}, \text{ despite} \quad (11)$$

$$E_{2,2} = 4\epsilon > 3\epsilon = E_{0,3}. \quad (12)$$

N-passivity

If we want to ensure that our notion of equilibrium does not collapse once we start combining systems we can impose the additional requirement that the combination of a number N of identical passive systems as

- $\rho_N = \bigotimes_k^N \pi^{(k)}$, and
- $H_N = \sum_{k=1}^N H^{(k)} \otimes_{l \neq k} \mathbf{I}^{(l)}$

still be passive. Here, k labels the N identical systems with reference Hamiltonians $H^{(k)} = H$. If ρ_N is passive with respect to H_N , π is called *N-passive*. We refer to states which are not *N-passive* as *N-active*.

In order to obtain a criterion for N-passivity, we consider passivity condition (2) for ρ_N . Comparing two energy levels of H_N , $E_a = \sum a_j \epsilon_j$ and $E_b = \sum b_j \epsilon_j$ with $\sum a_j = \sum b_j = N$, condition (2) for ρ_N reads¹:

$$\sum a_j \epsilon_j < \sum b_j \epsilon_j \Rightarrow \prod r_j^{a_j} \geq \prod r_j^{b_j}. \quad (13)$$

(We use the convention that $0^0 = 1$ and $0^n = 0$ for $n \in \mathbb{N}$). Since the logarithm is a monotonic function we may equally express the inequality on the right in terms of sums

$$\sum a_j \epsilon_j < \sum b_j \epsilon_j \Rightarrow \sum a_j \log r_j \geq \sum b_j \log r_j. \quad (14)$$

(For $r_j = 0$ take the limit $\lim_{r_j \rightarrow 0} \log r_j = -\infty$).

¹Convince yourself that any energy level of the N -partite system can be written in the form of E_a (or E_b) and that the right hand side expressions of Eq. 13 indeed equate the corresponding populations.

Complete passivity

If a state π remains N -passive in the limit $N \rightarrow \infty$ it is called *completely passive*.

In the following section we show that any state which is completely passive must either have Gibbs form (i.e., Eq. 1), or be the ground state.

II Proof of equivalence between complete passivity and thermality (optional)

We state this proof for completeness here. It is instructive but not required for the remainder of this course. We proceed as follows:

- 1) Note that (i) ground states are passive; (ii) the combination of ground states again results in a ground state; (iii) all other passive states have at least two populated levels.
- 2) We re-formulate Eq. 14 for three energy levels^a and a choice of N -partite energies.
- 3) We introduce *virtual temperatures* and show that they are the same for each transition if and only if the state has Gibbs form (Eq. 1).
- 4) For a passive (but non-thermal) state π , we choose two transitions with different virtual temperatures in order to show in general how any such state may be activated by system composition – i.e., $\pi^{\otimes N}$. This is done by explicit construction of two N -partite levels with population inversion that violate the condition obtained in step (2).

This completes the first part of the proof:

Any passive, non-Gibbs state may be activated.

- 5) In the last step we show the inverse – i.e.,

all Gibbs states γ_β remain thermal (and consequently, passive) under system composition – $\gamma_\beta^{\otimes N}$,

hence completing the proof.

^aConvince yourself that all passive qubit states are thermal. Passive but non-thermal states can consequently only exist in systems of at least three dimensions.

(2) First, we reformulate the conditions imposed by Eq. 14 for two specific energy levels E_a and E_b of an N -partite system where the first one, $E_a = a\epsilon_0 + (N - a)\epsilon_m$, consists of the single system levels ϵ_0 and ϵ_m . The second one is simply given by $E_b = N\epsilon_l$. For this choice of energy levels, we can express Eq. 14 as

$$a\epsilon_m + (N - a)\epsilon_0 < N\epsilon_l \Rightarrow a \log r_m + (N - a) \log r_0 \geq N \log r_l, \quad (15)$$

or, equivalently (assuming $r_0 \neq r_l$),

$$\frac{a}{N} \frac{\epsilon_m - \epsilon_0}{\epsilon_l - \epsilon_0} < 1 \Rightarrow \frac{a}{N} \frac{\log r_0 - \log r_m}{\log r_0 - \log r_l} \leq 1. \quad (16)$$

For an N -partite system whenever the condition on the left hand side of Eq. 16 holds for three energy levels, the right hand side has to be fulfilled for the same three levels. Otherwise, the state in question is N -active. The same holds for the inverse relationship (i.e., with inequality signs turned around). In part (4) we will use this condition to show that any passive state that is not thermal can be activated for some choice of a and N . First, we also need to introduce virtual temperatures.

(3) For any passive state π and any transition between non-degenerate levels ϵ_k and ϵ_l of the corresponding single-system reference Hamiltonian H the virtual temperature β_{kl} is defined as

$$\beta_{kl} := \frac{\log r_k - \log r_l}{\epsilon_l - \epsilon_k}. \quad (17)$$

Convince yourself that for a thermal state γ_β , $\beta_{k,l} = \beta \forall k, l$.

Conversely, for any passive, non-thermal state there are at least two transitions which do not share the same virtual temperature. This follows from the fact that for a passive state the relationship

$$\frac{r_n}{r_m} = \exp[-\beta(\epsilon_n - \epsilon_m)], \quad (18)$$

in addition to requiring the state to be normalised, in fact fully defines a thermal state (given β and reference Hamiltonian H).

Concretely, we may first choose the transition between the ground level ϵ_0 and any higher energy level and then look for a second transition with the ground state that has a different virtual temperature. For the two non-ground levels we may always choose the labels l and m such that $\epsilon_0 < \epsilon_l < \epsilon_m$ is fulfilled. We also assume $\epsilon_0 \geq 0$ without loss of generality.

(4) Having chosen two transitions in this way, we either have $\beta_{0l} < \beta_{0m}$ or $\beta_{0l} > \beta_{0m}$. In the following we consider the first case (and skip the second which is completely analogous):

$$\beta_{0l} < \beta_{0m} \quad (19)$$

$$\frac{\log r_0 - \log r_l}{\epsilon_l - \epsilon_0} < \frac{\log r_0 - \log r_m}{\epsilon_m - \epsilon_0} \quad (20)$$

Rearranging (again assuming $r_0 \neq r_l$):

$$\frac{\epsilon_m - \epsilon_0}{\epsilon_l - \epsilon_0} < \frac{\log r_0 - \log r_m}{\log r_0 - \log r_l} \quad (21)$$

$$(22)$$

We can multiply both sides by the ratio of two natural numbers a and N :

$$\frac{a}{N} \frac{\epsilon_m - \epsilon_0}{\epsilon_l - \epsilon_0} < \frac{a}{N} \frac{\log r_0 - \log r_m}{\log r_0 - \log r_l} \quad (23)$$

Now we can always choose $a < N$ such that the left-hand side of Eq. 23 is smaller than 1 while the right-hand side is larger, hence violating the condition for complete passivity imposed by Eq. 16. In other words, we may always find two N -partite levels, $E_a = a\epsilon_0 + (N - a)\epsilon_l$ and $E_b = N\epsilon_m$, which show population inversion for some possible choice of a and N . With this procedure, any given passive state π which is not thermal may be activated.

Note that the same construction is not possible for a thermal state, where the virtual temperatures between all transitions are the same because Eq. 19 does not hold for any transitions in that case. Even so, we still need to prove that thermal states cannot be activated (by some other procedure). This is done in step (5) by showing that $\gamma_\beta^{\otimes N}$ is thermal (and hence passive) for any N .

First, however, we clarify some special cases. r_0 and r_l can always be chosen non-zero and unequal unless the state is maximally mixed in which case it is already thermal (in the limit $\beta \rightarrow 0$). That leaves the case where $r_m = 0$. In this case we may directly invoke Eq. 13 and restate Eq. 15:

$$a\epsilon_m + (N - a)\epsilon_0 < N\epsilon_l \Rightarrow r_m^a r_0^{N-a} \geq r_l^N. \quad (24)$$

Choosing $a = 1$, the condition on the left may always be fulfilled for some N while the inequality on the right becomes $0 \geq r_l^N$ and can never be fulfilled for $r_l > 0$. Hence, the state may always be activated, as in the general case.

(5) It is straightforward to see, using multinomial expansion, that any combination of N identical thermal states is in turn thermal:

$$\begin{aligned}
\gamma_{\beta}^{\otimes N} &= \frac{1}{Z^N} \left[\sum_k e^{-\beta \epsilon_k} |\epsilon_k\rangle \langle \epsilon_k| \right]^{\otimes N} \\
&= \frac{1}{Z^N} \sum_{\mathbf{m}} \exp[-\beta \sum_{k=1}^d m_k \epsilon_k] \sum_{\mu_m} |E_m, \mu_m\rangle \langle E_m, \mu_m| \\
&= \frac{1}{Z^{(N)}} \sum_{\mathbf{m}, \mu_m} e^{-\beta E_m} |E_m, \mu_m\rangle \langle E_m, \mu_m|,
\end{aligned} \tag{25}$$

where the first sum in the second line goes over all combinations \mathbf{m} of m_k which sum to N : $\sum_{k=1}^d m_k = N$. d is the subsystem dimension. The states $|E_m, \mu_m\rangle$ correspond to the eigenenergies $E_m = \sum_{k=1}^d m_k \epsilon_k$ of the N -body Hamiltonian H_N . Each energy E_m is degenerate with a multiplicity equal to the multinomial coefficient

$$\binom{N}{m_1, m_2, \dots, m_d} := \frac{N!}{m_1! m_2! \dots m_d!}, \tag{26}$$

and eigenstates in the degenerate subspaces are labelled by μ_m . It is easy to see that Eq. 25 indeed represents a thermal state with $Z^{(N)} = Z^N$.

This concludes the proof that a passive state π is completely passive if and only if it is thermal.

We have now derived the emergence of the thermal distribution from a requirement of local equilibrium – passivity – and combination of identical, non-interacting systems. Remarkably these two requirements, local equilibrium and system combination, turn out to be sufficient to uniquely single out the Gibbs distribution of the thermal state.

This covers our introduction of the thermal state. In the next lectures we will discover and explore the resource theory of athermality whose free states are thermal states at a fixed ambient temperature.