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Lecture 5: Quantum Gibbs States

**September 18, 2025** *Scribe: Harry Putterman*

# 1 Quantum Gibbs States

**Definition 1.1.** Quantum Gibbs state: For a hamiltonian $H$ the Gibbs state at inverse temperature $\beta = \frac{1}{T}$ is defined as

$$\rho_\beta(H) = \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})} \tag{1}$$

We are interested in the quantum Gibbs state in the setting where the Hamiltonian is local, meaning that $H = \sum_\alpha b_\alpha P_\alpha$ where the $P_\alpha$ are Pauli operators with bounded support. Gibbs states appear in many circumstances across physics and computer science which we now briefly remark on.

### 1.0.1 Scenario 1

We have a system and have access to observables such as pressure, net charge, etc. Each observable corresponds to an operator $O_i$ and yields expected measurement outcomes $\mathrm{Tr}(O_i, \rho) = e_i$. We can interpret the measurements using the maximum entropy principle which says that the state should be the one the maximum possible entropy consistent with the measurements. That turns out to be the Gibbs state which takes the form

$$\rho = \frac{e^{-\sum_i \lambda_i O_i}}{Tr(e^{-\sum_i \lambda_i O_i})} \tag{2}$$

## 1.1 Scenario 2

We have a system with Hamiltonian $H_S$ coupled to an environment with Hamiltonian $H_E$ through the coupler Hamiltonian $H_{SE}$. The overall Hamiltonian is given by $H = H_S + H_E + \lambda H_{SE}$ where $\lambda \ll \|H_S\|, \|H_E\|$. If the initial state of our system is $\rho \otimes \rho_E$ after evolution under this Hamiltonian for some time $t$ the state of the system will be $\rho \otimes \rho_E \to e^{iHt}(\rho \otimes \rho_E)e^{-iHt}$. If we trace out state of the environment and make the assumption that the state of the environment is not affected by the evolution we will find that this evolution corresponds to some quantum channel $\epsilon_t(\rho)$. We can ask what the fixed point of this quantum channel is. It turns out that the fixed point is the Gibbs state. This channel is often called the Davies channel.

## 1.2 Scenario 3

In this setting we have some variables $x_1, ...., x_n$ and some constraint relations between variables represented by a dependency graph. A state $\rho$ which captures these dependencies is given by a Gibbs state (This is known as the Hammersley-Clifford theorem). In the quantum case the Hamiltonian corresponding to the Gibbs state is commuting.

### 1.3 Scenario 4

We have a Hamiltonian $H$ for our complete system defined on some lattice. The system is in an eigenstate $|\psi\rangle$ of this Hamiltonian satisfying $H|\psi\rangle = E|\psi\rangle$. What state describes a subsystem of the lattice $S$? This is also the Gibbs state

$$\rho_s = \frac{e^{-\beta H_S}}{\mathrm{Tr}(e^{-\beta H_s})} \tag{3}$$

where $H_s$ is $H$ restricted to the subsystem $S$ and $\beta$ is chosen so the energy of the Gibbs state matches the energy of $|\psi\rangle$. This is referred to as the eigenstate thermalization hypothesis (ETH).

## 2 Partition Function

**Definition 2.1.** The partition function $Z_\beta(H)$ is given by

$$Z_\beta(H) = \mathrm{Tr}(e^{-\beta H}) \tag{4}$$

Many useful quantities can be computed from the partition function. For example we can compute the expected value of a specific term in the Hamiltonian $H = \sum_\alpha b_\alpha P_\alpha$ using the following

$$\langle P_a \rangle = -\frac{1}{\beta}\frac{\partial}{\partial b_\alpha}\log(Z_\beta(H)) = -\frac{1}{\beta}\frac{\mathrm{Tr}(\frac{\partial}{\partial b_\alpha}e^{-\beta H})}{Z_\beta(H)} = \frac{\mathrm{Tr}(P_\alpha e^{-\beta H})}{Z_\beta(H)} = \mathrm{Tr}(P_\alpha \rho_\beta(H)). \tag{5}$$

(Note that in general it does *not* hold that $\frac{\partial}{\partial b_\alpha}e^{-\beta H} = -\beta P_\alpha e^{-\beta H}$, since the different $P_\alpha$s do not commute with each other. Nevertheless this equality holds under the trace, as shown in the appendix of these notes.) Next, let's use the partition function to study phase transitions with a specific model.

### 2.1 Curie-Weiss Model

This Hamiltonian for the Curie-Weiss model is

$$H = -\frac{1}{2n}\left(\sum_i Z_i\right)^2 - h\left(\sum_i Z_i\right) \tag{6}$$

We are interested in computing the magnetization, which is given by $M_{avg} = \frac{1}{n}\mathrm{Tr}\left((\sum_i Z_i)\rho_\beta(H)\right)$. To this end, let's compute the partition function:

$$\begin{aligned}
Z_\beta(H) &= \mathrm{Tr}\Big(e^{-\beta H}\Big) && (7)\\
&= \sum_{z\in\{0,1\}^n} \exp\left\{\frac{\beta}{2n}\left(n-2|Z|\right)^2 + \beta h\left(n-2|Z|\right)\right\} && (8)\\
&= \sum_{k=-n}^{n}\binom{n}{\frac{n+k}{2}}\exp\left[\frac{\beta}{2n}k^2 + \beta h\, k\right] && (9)\\
&\approx \sum_{k=-n}^{n}\exp\left\{n\, H\Big(\tfrac{1}{2}+\tfrac{k}{2n}\Big) + \frac{\beta}{2n}k^2 + \beta h\, k\right\} && (10)\\
&\approx \sum_{\delta\in[-1,1]}\exp\left\{n\left[H\Big(\tfrac{1+\delta}{2}\Big) + \tfrac{\beta}{2}\delta^2 + \beta h\,\delta\right]\right\}. && (11)
\end{aligned}$$

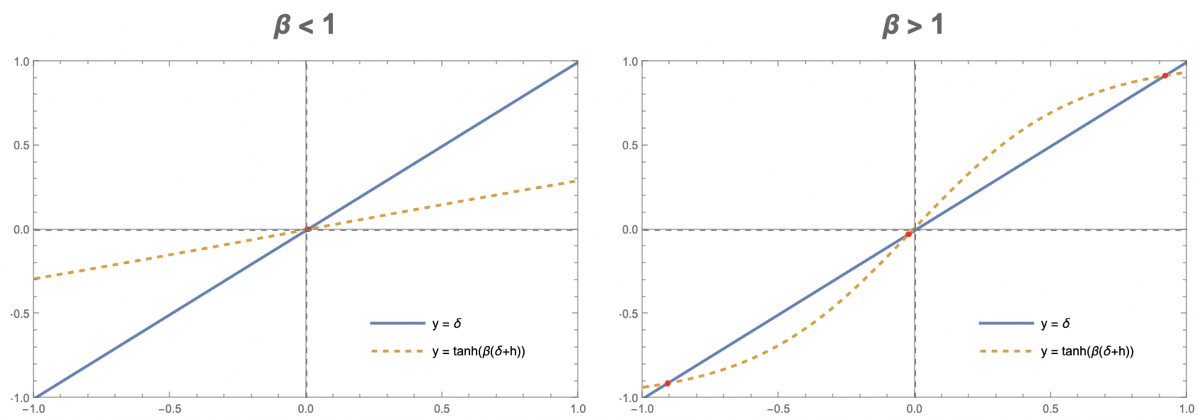


Figure 1: Magnetization phase transition

Now we can approximate the function by choosing the value of $\delta$ that maximizes the function. To find the $\delta^*$ which maximizes this expression we must solve the equation

$$\delta^* = \tanh\left(\beta(\delta^* + h)\right) \tag{12}$$

At the value $\delta^*$ the magnetization is given by

$$M_{avg} = -\frac{1}{\beta n}\frac{\partial}{\partial h}\log(\mathrm{Tr}(e^{-\beta H})) = \delta^* \tag{13}$$

Now lets graphically look at the equation for $\delta^*$ to see that there is a phase transition. The plot is shown in 1. On the left we can see that for $\beta < 1$ there is no intersection of $\delta$ and $\tanh\left(\beta(\delta + h)\right)$ whereas for $\beta > 1$ there is an intersection for $\delta > 0$. This change in behavior of the magnetization is a phase transition.

# 3 Quantum Markov Chains

## 3.1 Classical Markov Chain

Before considering the quantum case lets discuss the classical Markov chain. Consider a simple undirected graph shown as shown in 2 where each vertex is a classical variable. Each edge in the graph represents some dependency between the probability distribution of the vertices. For example in this graph we would have that $P(x_3, x_1|x_2) = P(x_3|x_2)P(x_1|x_2)$. In the classical setting when one has such a Markov property the state of the system can be represented as a Gibbs state of the form $P = e^{-\beta(H_{12}+H_{23}+H_{34}+H_{24})}$ (Clifford-Hammersley theorem).

## 3.2 Quantum Markov Chain

What is the quantum analog of the classical Markov chain? We can no longer think about conditional probabilities in the simple manner as the classical case. Consider a simple case with just three systems 1-2-3 connected in a linear chain.

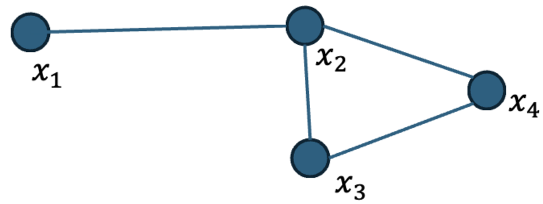


Figure 2: Dependency graph

**Definition 3.1.** Quantum Markov Chain: We say that $\rho_{123}$ for the system A-B-C is quantum Markov if $I(1:3|2) = I(1:23) - I(1:2) = 0$ where $I$ is the quantum mutual information.

**Theorem 3.2.** *Both directions of the same statement (presented for a situation with three systems coupled in a chain). [Petz] If $I(1:3|2) = 0$ that implies that the state of the system can be expressed as $\rho = e^{-\beta(H_{12}+H_{23})}/\mathrm{Tr}(e^{-\beta(H_{12}+H_{23})})$ where $[H_{12}, H_{23}] = 0$. [Kitaev-Viyalyi] If $\rho = e^{-\beta(H_{12}+H_{23})}$ where $[H_{12}, H_{23}] = 0$ then $\rho$ obeys the quantum Markov property.*

Let's understand each direction of the statement that the quantum Markov property is equivalent to being a Gibbs state of a commuting Hamiltonian. Petz showed that $I(1:3\,|\,2) = 0$ implies a decomposition

$$\rho_{123} = \bigoplus_b p_b \, \rho^b_{1,2_1} \otimes \rho^b_{2_3,3}. \tag{14}$$

One can then find a corresponding Hamiltonian

$$H = H_{12} + H_{23} \tag{15}$$

where the terms can be found to have the form

$$H_{12} = \bigoplus_b \Big( -\log \rho^b_{1,2_1} - \tfrac{1}{2} \log p_b \Big) \otimes I^b_{2_3}, \tag{16}$$

$$H_{23} = \bigoplus_b I^b_{2_1} \otimes \Big( -\log \rho^b_{2_3,3} - \tfrac{1}{2} \log p_b \Big). \tag{17}$$

The Gibbs state of this Hamiltonian reproduces $\rho_{123}$ and $[H_{12}, H_{23}] = 0$. For the other direction, if $\rho_{123} \propto e^{-(H_{12}+H_{23})}$ with $[H_{12}, H_{23}] = 0$, then one can find the Hamiltonians to be of the form (Bravyi–Vyalyi)

$$H_{12} = \bigoplus_b H^b_{1,2_1} \otimes I^b_{2_3}, \tag{18}$$

$$H_{23} = \bigoplus_b I^b_{2_1} \otimes H^b_{2_3,3}, \tag{19}$$

This then implies that $\rho_{123}$ satisfies the quantum Markov property.

An active area of research is studying the Gibbs state of a non-commuting Hamiltonian . Most of what we know for non-commuting Hamiltonians is in more restricted settings such as 1D.

## A Differentiating the partition function

Let $F(x)$ be a matrix-valued analytic function.

$$\begin{aligned}
\frac{d}{dx}\mathrm{Tr}[F(x)^k] &= \lim_{\delta\to 0}\frac{\mathrm{Tr}[F(x+\delta)^k]-\mathrm{Tr}[F(x)^k]}{\delta} && (20)\\
&= \lim_{\delta\to 0}\frac{1}{\delta}\mathrm{Tr}[(F(x)+\delta F'(x)+O(\delta^2))^k - F(x)^k] && (21)\\
&= \lim_{\delta\to 0}\frac{1}{\delta}\mathrm{Tr}[\delta(F(x)^{k-1}F'(x)+F(x)^{k-2}F'(x)F(x)+\dots)+O(\delta^2)] && (22)\\
&= k\mathrm{Tr}[F(x)^{k-1}F'(x)], && (23)
\end{aligned}$$

where we used the cyclicity of the trace in the last step. This mean that in particular,

$$\frac{d}{dx}\mathrm{Tr}[(Ax+B)^k] = k\mathrm{Tr}[(Ax+B)^{k-1}A]. \tag{24}$$

We may now use this to differentiate the matrix exponential.

$$\begin{aligned}
\frac{d}{dx}\mathrm{Tr}[e^{Ax+B}] &= \frac{d}{dx}\mathrm{Tr}\left[\sum_{t=0}^{\infty}\frac{1}{t!}(Ax+B)^t\right] && (25)\\
&= \sum_{t=1}^{\infty}\frac{1}{t!}\cdot t\mathrm{Tr}[(Ax+B)^{t-1}A] && (26)\\
&= \mathrm{Tr}\left[\sum_{t=1}^{\infty}\frac{1}{(t-1)!}(Ax+B)^{t-1}A\right] && (27)\\
&= \mathrm{Tr}[e^{Ax+B}A]. && (28)
\end{aligned}$$

This implies that

$$\frac{\partial}{\partial b_\alpha}\mathrm{Tr}[e^{-\beta\sum_\alpha b_\alpha P_\alpha}] = \mathrm{Tr}[(-\beta b_\alpha P_\alpha)\cdot e^{-\beta\sum_\alpha b_\alpha P_\alpha}], \tag{29}$$

as desired.