Deriving the Thermal Equilibrium State for a Finite Quantum Spin System

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Abstract

The aim of the lecture is to derive and study the Thermal Equilibrium State for a Finite Quantum Spin System. Which is defined as the state that minimize the Free Energy Functional. This state is called the Gibbs State and we will derive it by using the Variational Principle. Also, we will study the relation between it and the KMS condition.

1. The Gibbs State

The Energy is conservative and can be transformed from one form to another. but there are limitations on how the energy can be transformed. the energy may be in an ordered form like work or in a disordered form like heat. The maximum of the reversible work that may be performed by a thermodynamic system at certain conditions is defined as the free energy of the system (Thermodynamic potential) and it strongly depends on the entropy of the system. The state of the thermal equilibrium (The Gibbs state) is an equilibrium probability distribution which remains invariant under future evolution of the system which also can be defined as the minimizer of the free energy functional because of the second law of thermodynamics. In order to define the free energy functional $F(\rho)$ of a state defined by a density matrix ρ, let $\beta = (K_B T)^{-1} \in [0, \infty)$ is the inverse temperature, $H = H^* \in \mathcal{A} = B(\mathcal{H})$ is the Hamiltonian of a finite quantum spin system, and $S(\rho) = -Tr(\rho log(\rho)) \in [0, log(dim\mathcal{H})]$ is the Von Neumann's definition of entropy. Then the free energy functional is defined by:

$$F(\rho) = Tr(\rho H) - \beta^{-1} S(\rho) \quad (1)$$

Proposition 1. $\rho_\beta = Z(\beta)^{-1}e^{-\beta H}$ is the unique density matrix that minimize the free energy functional where $Z(\beta) = Tr(e^{-\beta H})$ is the partition function (normalization factor).

Now by using this proposition we can see that:

$$F(\rho_\beta) = Tr(\rho_\beta H) - \beta^{-1}S(\rho_\beta)$$

$$= Tr(e^{-\beta H}Z(\beta)^{-1}H) + \beta^{-1}Tr(e^{-\beta H}Z(\beta)^{-1}log(e^{-\beta H}Z(\beta)^{-1}))$$

$$= Tr(e^{-\beta H}Z(\beta)^{-1}H) + \beta^{-1}Tr(e^{-\beta H}Z(\beta)^{-1}log(e^{-\beta H}) - e^{-\beta H}Z(\beta)^{-1}log(Z(\beta)))$$

$$= -\beta^{-1}Tr(e^{-\beta H}Z(\beta)^{-1}log(Z(\beta))) = -\beta^{-1}Z(\beta)^{-1}log(Z(\beta))Tr(e^{-\beta H})$$

$$= -\beta^{-1}log(Z(\beta)) \tag{2}$$

The proof of the previous proposition follows by applying the following lemma.

Lemma 1. Let A and B be two non-negative definite matrices satisfying $0 \leq A, B \leq \mathbb{1}$ and such that $Ker(B) \subset Ker(A)$ then.

$$Tr(A(logA - LogB)) \geq Tr(A - B) + \frac{1}{2}Tr(A - B)^2 \tag{3}$$

Proof. The function $f(x) = -xlogx$, $x > 0$, continuously extended such that $f(0) = 0$, is easily seen to be concave. In fact $f \in C^2((0, \infty))$ with

$$f''(x) = -\frac{1}{x} \tag{4}$$

By Taylor Remainder Theorem, for $y > x$ there exist a ξ such that $x \leq \xi \leq y$ and

$$f(x) = f(y) + f'(y)(x - y) + \frac{f''(\xi)}{2}(x - y)^2$$

By the expression for f'' and for all x and y such that $0 \leq x \leq \xi \leq y \leq 1$

$$f(y) - f(x) + f'(y)(x-y) = -\frac{f''(\xi)}{2}(x-y)^2 = \frac{1}{2\xi}(x-y)^2 \geq \frac{1}{2}(x-y)^2 \quad (5)$$

As A and B are non-negative definite, they are diagonalizable. So, using the spectral decompositions of A and B, i.e.,

$$A = \sum_j a_j |\phi_j >< \phi_j| \quad (6)$$

$$B = \sum_i b_i |\psi_i >< \psi_i| \quad (7)$$

$$\sum_j |\phi_j >< \phi_j| = \sum_i |\psi_i >< \psi_i| = \mathbb{1} \quad (8)$$

So, we can see that

$$Tr(A(logA - logB)) - Tr(A-B) - \frac{1}{2}Tr(A-B)^2$$

$$= Tr(AlogA - AlogB - A + B - \frac{1}{2}(A-B)^2)$$

$$= Tr(-f(A) + A\frac{f(B)}{B} - A + B - \frac{1}{2}(A-B)^2 + f(B) - f(B))$$

$$= Tr(-f(A) + A(\frac{f(B)}{B} - 1) - B(\frac{f(B)}{B} - 1) + f(B) - \frac{1}{2}(A-B)^2)$$

$$= Tr(-f(A) + f(B) + (A-B)f'(B) - \frac{1}{2}(A-B)^2)$$

By multiplying by the Identity two times. And since any matrix commute with itself. And by using the cyclicity of the trace

$$= \sum_{ij} Tr(|\psi_i >< \psi_i||\phi_j >< \phi_j|[f(B) - f(A) + (A-B)f'(B) - \frac{1}{2}(A^2 + B^2 - 2AB)])$$

$$= \sum_{ij} Tr(|\psi_i >< \psi_i||\phi_j >< \phi_j|[f(b_i) - f(a_j) + (a_j - b_i)f'(b_i) - \frac{1}{2}(a_j - b_i)^2]) \geq 0$$

Where the last inequality follows from applying (5) term by term.
Now to prove Proposition 1, we can apply Lemma 1 with $A = \rho$, where ρ is an arbitrary density matrix, and $B = \rho_\beta$ ($KerB = 0$). This gives

$$\beta(F(\rho) - F(\rho_\beta)) = \beta Tr(\rho H) + Tr(\rho log\rho) + logZ(\beta)$$

$$= Tr(\rho\beta H) + Tr(\rho log\rho) + logZ(\beta)Tr(\rho)$$

$$= Tr(\rho log\rho) + Tr(\rho(\beta H + logZ(\beta)))$$

$$= Tr(\rho log\rho) - Tr(\rho log\frac{e^{-\beta H}}{logZ(\beta)})$$

$$= Tr(\rho(log\rho - log\rho_\beta)) \geq Tr(\rho - \rho_\beta) + \frac{1}{2}Tr(\rho - \rho_\beta)^2 = \frac{1}{2}Tr(\rho - \rho_\beta)^2 \geq 0$$

If the RHS vanishes, we have $\rho = \rho_\beta$. Hence the minimum of $F(\rho)$ is uniquely attained for $\rho = \rho_\beta$.

Also, we can study the Gibbs state for a certain Hamiltonian at the very high and low temperature limits which will be very useful to give us a sense about the interpretation of the Gibbs state. Let $H = H^* \in \mathcal{A} = B(\mathcal{H})$ is the Hamiltonian of a finite quantum spin system with eigenvectors $|1>, |2>, ..., |N>$ and eigenvalues $\lambda_1, \lambda_2, ..., \lambda_N$.

First we can start by the very high temperature limit ($\beta \to 0$)

$$\lim_{\beta \to 0} \rho_\beta = \frac{1}{dim\mathcal{H}}\mathbb{1}$$

This means that, all the energy eigenstates are equiprobable at $T \to \infty$.

For the very low temperature limit ($\beta \to \infty$) it's Little harder to find the limit, so, we will take the limit of the diagonal elements of ρ_β

$$\lim_{\beta \to \infty} < m|\rho_\beta|m >= \lim_{\beta \to \infty} \frac{1}{\sum_{n=1}^{N} e^{\beta(\lambda_m - \lambda_n)}} = \begin{cases} undefined & m = 1(ground\ state) \\ o & m > 1 \end{cases}$$

But we know that $Tr(\rho_\beta) = 1$. So, the limit for the ground state element should equal to 1. Which means only the ground state will be exist at that limit.

2. The Kubo-Martin-Schwinger Condition

Consider a finite dimensional Hilbert space $\mathcal{H}$, and a Hamiltonian $H = H^* \in \mathcal{A} = B(\mathcal{H})$. Denote the Heisenberg dynamics by τ_t. A state ω is called a β-KMS state if $\forall A, B \in \mathcal{A}$ it satisfies

$$\omega(A\tau_{i\beta}(B)) = \omega(BA) \tag{9}$$

Proposition 2. ω is a β-KMS $\iff$ $\omega = \omega_\beta$, i.e. , the KMS state coincides with the Gibbs state.

Proof. First, the KMS property of the Gibbs state.

$$\omega_\beta(A\tau_{i\beta}(B)) = Tr\rho_\beta Ae^{itH}Be^{-itH}|_{t=iB} = \frac{1}{Z(\beta)}Tre^{-\beta H}Ae^{-\beta H}Be^{\beta H}$$

$$= \frac{1}{Z(\beta)}Tre^{-\beta H}BA = Tr\rho_\beta BA = \omega_\beta(BA)$$

For the other direction, let $|1>, |2>, ..., |n>$ are the orthonormal basis of eigenvectors of H, with eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$. The KMS property of a state with density matrix ρ with $A = |i><j|$ and $B = |k><l|$ then

$$\omega(A\tau_{i\beta}(B)) = \omega(BA)$$

$$Tr\rho|i><j|e^{i(i\beta)H}|k><l|e^{-i(i\beta)H} = Tr\rho|k><l|i><j|$$

$$\sum_m <m|\rho|i><j|e^{-\beta\lambda_k}|K><l|e^{\beta\lambda_l}|m>=\sum_m <m|\rho|k><l|i><j|m>$$

$$<l|\rho|i>\delta_{jk}e^{\beta(\lambda_l-\lambda_k)} =<j|\rho|k>\delta_{li}$$

Since ρ is a density matrix it has at least one non-zero diagonal element. In fact, the last equation imply that ρ is diagonal in the basis of H. Let $l = i$ and $k = j$, we obtain that

$$<i|\rho|i>e^{\beta\lambda_i} = c$$

$$< i|\rho|i >= ce^{-\beta\lambda_i}$$

$$\rho = ce^{-\beta H}$$

Which is the definition of the Gibbs state.

It is important to note that, although these notions coincide in finite volume, it is not clear (from the beginning) that they also coincide in infinite volume. This requires proof.