Gibbs Variational Formula for Thermal Equilibrium States in Terms of Quantum Relative Entropy Density

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Abstract
We prove the Gibbs variational formula in terms of quantum relative entropy density that characterizes translation invariant thermal equilibrium states in quantum lattice systems. It is a natural quantum extension of the similar statement established by Föllmer for classical systems.

Keywords
Gibbs variational principle · Quantum Gibbs states · Quantum relative entropy

Mathematics Subject Classification
82B10 · 82B20 · 46L55

1 Introduction
Translation invariant thermal equilibrium states are identified with those attaining minimum free energy. This wisdom of statistical physics is called the Gibbs variational principle, and its rigorous mathematical formulation has been established for classical lattice systems [1] and quantum lattice systems [2].

The Gibbs variational principle can be expressed in terms of the relative entropy (Kullback–Leibler divergence [3]) as stated in [4] for classical systems. In this note, we establish an analogous statement for quantum lattice systems by extending the previous work [5] to a larger class of translation covariant potentials \( \Phi \). In more detail, we will prove that the information rate \( h(\omega \parallel \Phi, \beta) \) of any translation invariant state \( \omega \) with respect to the potential \( \Phi \) is equal to the relative entropy density \( h(\omega | \psi) \) of \( \omega \) with respect to any translation invariant thermal equilibrium state \( \psi \) for \( \Phi \). This equivalence immediately yields the complete characterization of translation invariant thermal equilibrium states \( \psi \) by the equality condition \( h(\varphi | \psi) = 0 \).

In [5] under the rather restricted setup that admits only a unique thermal equilibrium state \( \psi \), the equality \( h(\omega \parallel \Phi, \beta) = h(\omega | \psi) \) is verified. We prove this equality for a more general case that can have multiple thermal phases (induced by symmetry breaking). In the above...
sense, this paper makes a progress by relating quantum statistical physics to information theory. However, in terms of mathematics, we simply follow the argument invented by Hiai-Petz [5] using a recent finding by Ejima-Ogata [6].

2 Preliminaries

In this section we give our formulation that is based on C*-algebraic quantum statistical physics [7,8]. We will include a short review of some relevant ideas and known facts for the readers who are not familiar with them.

2.1 Quantum Relative Entropy

First we recall the quantum relative entropy by Umegaki [9]. It is a fundamental quantity of this paper. Consider any finite dimensional full matrix algebra $M_n(\mathbb{C}) (n \in \mathbb{N})$. Let $\text{Tr}$ denote the matrix trace which takes 1 on each one-dimensional projection. Let $\psi_1$ and $\psi_2$ be states on $M_n(\mathbb{C})$ whose density matrices with respect to $\text{Tr}$ are denoted by $D(\psi_1)$ and $D(\psi_2)$. The relative entropy of $\psi_1$ with respect to $\psi_2$ is given as

$$S(\psi_1 | \psi_2) = \begin{cases} \psi_1(\log D(\psi_1) - \log D(\psi_2)) & \text{if } \text{supp} \psi_1 \subseteq \text{supp} \psi_2 \\ +\infty & \text{otherwise.} \end{cases}$$ (1)

It is a quantum analogue of Kullback–Leibler divergence [3]. Note that for any state $\psi$ on $M_n(\mathbb{C})$ its von Neumann entropy $S(\psi)$ is given in terms of the quantum relative entropy as

$$S(\psi) \equiv \psi(-\log D(\psi)) = -S(\psi | \text{tr}) + \log n,$$ (2)

where $\text{tr}$ denotes the tracial state on $M_n(\mathbb{C})$ given as $\text{tr} = \frac{1}{n} \text{Tr}$.

2.2 Quantum Lattice Systems

We consider a quantum spin lattice system on a cubic lattice $\mathbb{Z}^v$ of arbitrary dimension $v \in \mathbb{N}$. For any subset $A \subset \mathbb{Z}^v$ let $|A|$ denote the number of sites in $A$, where $|A|$ will be identified with the volume of $A$. The notation $A \in \mathbb{Z}^v$ means that $A$ is a subset of $\mathbb{Z}^v$ with finite volume $|A| < \infty$. Let $\mathfrak{H}_{\text{loc}} := \{ \Lambda ; \ A \in \mathbb{Z}^v \}$, the set of all finite subsets of $\mathbb{Z}^v$.

Fix any $n \in \mathbb{N}$. Let $\mathcal{H}_n$ denote the Hilbert space of the dimension $n \in \mathbb{N}$. To each site $x \in \mathbb{Z}^v$ we assign the same Hilbert space $\mathcal{H}_n$ which will be written as $\mathcal{H}_x$ by specifying the site. For any finite subset $A \subset \mathbb{Z}^v$ the Hilbert space associated to $A$ is given by $\mathcal{H}_A := \bigotimes_{x \in A} \mathcal{H}_x$. The local algebra $\mathcal{A}(A)$ on $A$ is given by the $|A|$-fold tensor product of $M_n(\mathbb{C})$, and hence $\mathcal{A}(A) \simeq M_{|A|}(\mathbb{C})$. If $A \subset A' \subset \mathbb{Z}^v$, then $\mathcal{H}_{A'} = \mathcal{H}_A \otimes \mathcal{H}_{A \setminus A}$. We embed $\mathcal{A}(A)$ into $\mathcal{A}(A')$ by identifying $A \in \mathcal{A}(A)$ with $A \otimes 1_{A \setminus A} \in \mathcal{A}(A')$, where $I$ denotes the identity operator. Let $\mathfrak{A}_{\text{loc}} := \bigcup_{A: A \in \mathfrak{H}_{\text{loc}}} \mathcal{A}(A)$ to which the operator-norm is naturally assigned. The norm-completion of $\mathfrak{A}_{\text{loc}}$ yields a quasi-local C*-algebra $\mathfrak{A}$. The dense subalgebra $\mathfrak{A}_{\text{loc}}$ in $\mathfrak{A}$ will be called the local algebra. The identity element of $\mathfrak{A}$ is denoted by $1$. Let $\mathfrak{A}_{\text{sa}} := \{ A \in \mathfrak{A} ; \ A = A^* \}$, i.e. the set of self-adjoint elements of $\mathfrak{A}$. For any $A \subset \mathbb{Z}^v$ define $\mathcal{A}_{A} = \mathfrak{A}_{A} \cap \mathfrak{A}_{\text{sa}}$. The space-translation group of automorphisms on $\mathfrak{A}$ is denoted by $\{ \gamma_x ; \ x \in \mathbb{Z}^v \}$. It satisfies the covariance relation $\gamma_x (\mathcal{A}(A)) = \mathcal{A}(A + x)$ for every $x \in \mathbb{Z}^v$ and $A \subset \mathbb{Z}^v$. 

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The quantum spin model can be specified by a potential $\Phi$ as follows. Let $\Phi$ be a map $\mathcal{F}_{\text{loc}} \mapsto \mathcal{A}_{\text{loc}}$ such that for any $\Lambda \in \mathcal{F}_{\text{loc}}$

$$\Phi(\Lambda) \in \mathcal{A}(\Lambda)_{sa},$$

(3)

and that for any $x \in \mathbb{Z}^n$ and $\Lambda \in \mathcal{F}_{\text{loc}}$

$$\Phi(\Lambda + x) = \gamma_x(\Phi(\Lambda)).$$

(4)

By (3) $\Phi(\Lambda)$ gives an interaction among all the sites in $\Lambda$. By (4) $\Phi$ gives a translation invariant model. The internal energy on $\Lambda \in \mathcal{F}_{\text{loc}}$ is given as

$$U_\Lambda := \sum_{X \subset \Lambda} \Phi(X) \in \mathcal{A}(\Lambda)_{sa}.$$  

(5)

The surface energy $W_\Lambda$ of $\Lambda \in \mathcal{F}_{\text{loc}}$ may be given by the summation of all the interactions on the surface of $\Lambda$:

$$W_\Lambda := \sum_{X \in \mathcal{F}_{\text{loc}} : X \cap \Lambda \neq \emptyset, X \cap \Lambda^c \neq \emptyset} \Phi(X) \in \mathcal{A}_{sa}.$$  

(6)

We assume the existence of $W_\Lambda \in \mathcal{A}_{sa}$ for any $\Lambda \in \mathcal{F}_{\text{loc}}$. For each $\Lambda \in \mathcal{F}_{\text{loc}}$ let

$$H_\Lambda := U_\Lambda + W_\Lambda \in \mathcal{A}_{sa}.$$  

(7)

For any $I \in \mathcal{F}_{\text{loc}}$, one can uniquely define the linear map from $\mathcal{A}(I)$ to $\mathcal{A}$ by

$$\delta_\Phi(A) = i[H_I, A], \quad A \in \mathcal{A}(I),$$

(8)

where $J \in \mathcal{F}_{\text{loc}}$ is any finite subset such that $J \supset I$. By the set of consistent equations (8) for all $I \in \mathcal{F}_{\text{loc}}$ we can uniquely determine a $*$-derivation $\delta_\Phi$ on the domain $\mathcal{A}_{\text{loc}}$. Assume the existence of the strongly continuous one-parameter group of $*$-automorphisms $\alpha_t (t \in \mathbb{R})$ of $\mathcal{A}$ whose infinitesimal is given by

$$\frac{d}{dt} \alpha_t(A) \bigg|_{t=0} = \delta_\Phi(A), \quad A \in \mathcal{A}_{\text{loc}}.$$  

(9)

This one-parameter group of $*$-automorphisms $\alpha_t (t \in \mathbb{R})$ denotes a quantum time evolution of the infinitely extended quantum system $\mathcal{A}$ determined by the translation covariant potential $\Phi$. Finally, we put the following crucial assumption:

$$\lim_{\Lambda \to \infty} \frac{\|W_\Lambda\|}{|\Lambda|} = 0,$$

(10)

where $\Lambda \to \infty$ means the van Hove limit [10]. This standard assumption says that the ratio of the norm of the surface energy to the volume of the specified region will vanish in the thermodynamic limit.

We will give notations about states. Let $\omega$ be a state (i.e. normalized positive linear functional) of $\mathcal{A}$. For any subset $\Lambda \subset \mathbb{Z}^n$, $\omega_\Lambda$ denotes the restriction of $\omega$ to $\mathcal{A}(\Lambda)$:

$$\omega_\Lambda(A) = \omega(A) \quad \forall \Lambda \in \mathcal{A}(\Lambda).$$

(11)

For each $\Lambda \in \mathcal{F}_{\text{loc}}$ the density matrix $D_\Lambda$ for $\omega$ is determined by

$$\omega_\Lambda(A) = \text{Tr}_A(D_\Lambda A) \quad \forall \Lambda \in \mathcal{A}(\Lambda),$$

(12)

where $\text{Tr}_A$ denotes the matrix trace of $\mathcal{A}(\Lambda)$. A state $\omega$ on $\mathcal{A}$ is translation invariant if

$$\omega(\gamma_x(A)) = \omega(A) \quad \forall A \in \mathcal{A}, \forall x \in \mathbb{Z}^n.$$  

(13)
We denote the set of all states on $\mathcal{A}$ by $S(\mathcal{A})$, and the set of all translation invariant states by $S_T(\mathcal{A})$.

For any state $\omega$ of $\mathcal{A}$ the triplet $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ denotes its GNS representation [7]. Namely $\pi_\omega$ is a $*$-representation of the algebra $\mathcal{A}$ on the Hilbert space $\mathcal{H}_\omega$, and $\Omega_\omega \in \mathcal{H}_\omega$ is a normalized cyclic vector such that $\omega(A) = (\Omega_\omega, \pi_\omega(A)\Omega_\omega)$ for all $A \in \mathcal{A}$. The GNS representation yields a von Neumann algebra $\mathcal{M}_\omega := \pi_\omega(\mathcal{A})''$ on $\mathcal{H}_\omega$, where $''$ denotes the double commutant. The commutant algebra is given by $\mathcal{M}_\omega' := \{X \in \mathcal{B}(\mathcal{H}_\omega); \ [X, Y] \equiv XY - YX = 0 \ \forall Y \in \mathcal{M}_\omega\}$ and the center is given by $\mathcal{Z}_\omega := \mathcal{M}_\omega \cap \mathcal{M}_\omega'$. A state $\omega$ of $\mathcal{A}$ is called a factor state if its center is trivial, i.e. $\mathcal{Z}_\omega = \mathbb{C}I$, where $I$ denotes the identity operator in $\mathcal{H}_\omega$. A factor state corresponds to a pure thermal phase.

### 2.3 Thermal Equilibrium States

We introduce several notions of thermal equilibrium for quantum systems (which turn out to be equivalent under certain conditions). First we recall the Kubo–Martin–Schwinger (KMS) condition [11–13] which is the most fundamental one among others, see the monograph [7,8].

**Definition 1 (KMS condition)** Let $\alpha_t$ $(t \in \mathbb{R})$ be a (strongly continuous) one-parameter group of $*$-automorphisms of $\mathcal{A}$. For $\beta > 0$ define the strip region $D_\beta := \{z \in \mathbb{C}; 0 \leq \text{Im}z \leq \beta\}$ in the complex plane $\mathbb{C}$ and its interior $\overset{\circ}{D}_\beta$. A state $\varphi$ of $\mathcal{A}$ is called an $\alpha_t$-KMS state at inverse temperature $\beta \in \mathbb{R}$ or $(\alpha_t, \beta)$-KMS state if it satisfies the following set of conditions:

1. $F_{A, B}(z)$ is analytic in $\overset{\circ}{D}_\beta$,
2. $F_{A, B}(z)$ is continuous and bounded on $D_\beta$,
3. For all $t \in \mathbb{R}$, $F_{A, B}(t) = \varphi(A\alpha_t(B))$, $F_{A, B}(t + i\beta) = \varphi(\alpha_t(B)A)$.

The set of all $(\alpha_t, \beta)$-KMS states is denoted as $S^{\text{KMS}}(\omega, \beta)(\mathcal{A})$.

Let $\varphi$ be a KMS state and $(\mathcal{H}_\varphi, \pi_\varphi, \Omega_\varphi)$ denote its GNS representation. Then the cyclic vector $\Omega_\varphi \in \mathcal{H}_\varphi$ automatically becomes a separating vector for the von Neumann algebra $\mathcal{M}_\varphi$, i.e. $X\Omega_\varphi = 0$ for $X \in \mathcal{M}_\varphi$ implies $X = 0$. Let $\Delta_\varphi$ denote the modular operator for $(\mathcal{M}_\varphi, \Omega_\varphi)$ of Tomita–Takesaki modular theory [7]. Let $\tilde{\varphi}$ denote the state extension of $\varphi$ to $\mathcal{M}_\varphi$ given by $\tilde{\varphi}(X) = (\Omega_\varphi, X\Omega_\varphi)$ for $X \in \mathcal{M}$. It satisfies the KMS condition for the modular automorphism group $\sigma_t := \text{Ad}(\Delta_\varphi^{it})$ $(t \in \mathbb{R})$ at the inverse temperature $\beta = -1$. (This minus sign of $\beta$ requires obvious change in Definition 1.)

Based on the above KMS condition with Tomita–Takesaki modular theory, another somewhat technical characterization of thermal equilibrium was given in [14,15]. We call it the Araki–Ion quantum Gibbs condition, or the AI Gibbs condition. The AI Gibbs condition rigorously defines “Gibbs states” for quantum systems, and it is manifestly reduced to the DLR condition [16,17] for classical interactions. Let $\varphi$ be a state that has its cyclic and separating GNS vector $\Omega_\varphi \in \mathcal{H}_\varphi$. Following [18] define

$$\Omega_\varphi(V) := \exp \left( \frac{\log \Delta_\varphi + V}{2} \right) \Omega_\varphi$$

$$= \sum_{m=0}^{\infty} \int_0^1 \frac{1}{d^1} \int_0^{t_1} \cdots \int_0^{t_{m-1}} \int_0^{t_m} \Delta_\varphi^{t_m} \cdot V \Delta_\varphi^{t_{m-1}-t_m} \cdot V \cdots \Delta_\varphi^{t_1-t_2} \cdot V \Omega_\varphi$$
\[ \equiv \text{Exp}_r \left( \int_0^{\frac{1}{2}} : A_\psi^t V \Delta_\psi^{-t} dt \right) \Omega_\psi, \quad (14) \]

where the sum converges absolutely, and the notation \( \text{Exp}_r \) denotes the Dyson time-ordering expansion \[19\]. If \( V = \pi_\psi(h) \) for \( h \in \mathcal{A}_{sa} \), we denote the perturbed vector simply by \( \Omega_\psi(h) \). Then we obtain the positive linear functional and the state on \( \mathcal{A} \) generated by this new vector as

\[ \varphi^h(A) := (\Omega_\psi(h), \pi_\psi(A) \Omega_\psi(h)) \quad A \in \mathcal{A}, \quad (15) \]

\[ [\varphi^h](A) := \frac{(\Omega_\psi(h), \pi_\psi(A) \Omega_\psi(h))}{\langle \Omega_\psi(h), \Omega_\psi(h) \rangle} = \frac{\varphi^h(A)}{\varphi^h(1)} \quad A \in \mathcal{A}. \quad (16) \]

The weak extensions of \( \varphi^h \) and \([\varphi^h]\) to \( \mathcal{M}_\varphi \) will be denoted by the same notation, as there seems no fear of confusion.

**Definition 2** (Araki-Ion quantum Gibbs condition) Assume a (not necessarily translation covariant) potential \( \Phi \) that generates a (strongly continuous) one-parameter group of \( \ast \)-automorphisms of \( \mathcal{A} \). Let \( \varphi \) be a state of \( \mathcal{A} \) and \((H_\varphi, \pi_\varphi, \Omega_\varphi)\) denote its GNS triplet. The state \( \varphi \) is called a Gibbs state for \( \Phi \) at \( \beta \) or a \((\Phi, \beta)\)-Gibbs state if it satisfies

(i) its GNS vector \( \Omega_\varphi \) is separating for \( \mathcal{M}_\varphi \),

(ii) its perturbed state by \( \beta W_A \) has the following product form

\[ [\varphi^{\beta W_A}](AB) = \rho^{IG}_A(\varphi^{\beta W_A})(B), \quad A \in \mathcal{A}(\Lambda), \quad B \in \mathcal{A}(\Lambda^c), \quad (17) \]

where \( \rho^{IG}_A \) denotes the internal canonical Gibbs state on \( \mathcal{A}(\Lambda) \) determined by the internal energy \( U_\Lambda \) with respect to the potential \( \Phi \) as

\[ \rho^{IG}_A(\varphi) = \frac{\text{Tr}_A(A e^{-\beta U_\Lambda})}{\text{Tr}_A(e^{-\beta U_\Lambda})}, \quad A \in \mathcal{A}(\Lambda). \quad (18) \]

Let \( \mathcal{S}^{\text{Gibbs}}(\mathcal{A}, \Phi, \beta) \) denote the set of all \((\Phi, \beta)\)-Gibbs states.

**Remark 1** In the product formula (17) the state on the specified local system \( \mathcal{A}(\Lambda) \) is given by the internal canonical Gibbs state \( \rho^{IG}_A \) uniquely determined by the interactions in \( \Lambda \). \( \rho^{IG}_A \) should not be confused with the restriction of an AI Gibbs state \( \varphi \) to \( \mathcal{A}(\Lambda) \), which can not be explicitly given unless the potential \( \Phi \) is trivial. (Bratteli-Robinson’s notation and ours are different; \( \omega_\Lambda \) in Definition 6.2.16 \[8\] means the above \( \rho^{IG}_A \), not \( \omega|_{\mathcal{A}(\Lambda)} \).)

From now on we focus on the translation-invariant case, i.e. only translation invariant states for a translation covariant potential. We will define thermodynamic functions that are basic ingredients of thermodynamic formalism \[8,20\]. The pressure is defined as the following thermodynamic limit (the van Hove limit):

\[ P(\Phi) := \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \log \text{Tr}_A(e^{-U_\Lambda}). \quad (19) \]

For any translation invariant state \( \omega \) of \( \mathcal{A} \), the energy density is given by

\[ e_{\Phi}(\omega) := \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \omega(U_\Lambda), \quad (20) \]

and the entropy density is given by

\[ s(\omega) \equiv \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} S(\omega_\Lambda). \quad (21) \]
The strong subadditivity of quantum entropy [23] is known to yield the existence of \( s(\omega) \) and its some properties [24]. To guarantee \( P(\Phi) \) and \( e_{\Phi}(\omega) \) we require a certain decay condition for the translation covariant potential \( \Phi \). We shall come back to this point later.

With the thermodynamic quantities we have the following variational formula:

\[
P(\beta \Phi) = \sup_{\omega \in \mathcal{S}_{\gamma}^0} \left\{ s(\omega) - \beta e_{\Phi}(\omega) \right\}.
\] (22)

The quantity \( s(\omega) - \beta e_{\Phi}(\omega) \) in the right-hand side is the free energy of the state \( \omega \) multiplied by the minus constant \(-\beta\); that is why we use \( \sup \) rather than \( \inf \). The variational formula characterizes thermal equilibrium as the minimum free-energy condition [1]: A translation invariant state \( \varphi \) is called a thermal equilibrium state if it takes the supremum of (22):

\[
P(\beta \Phi) = s(\varphi) - \beta e_{\Phi}(\varphi).
\] (23)

It has been known for some time that the variational principle (22) can be verified by using quantum relative entropy as follows, see [8]. First we note the following identity for any \( \Lambda \in \mathfrak{F}_{\text{loc}} \):

\[
S(\omega_\Lambda|\rho^\text{IG}_\Lambda) = -s(\omega_\Lambda) + \beta \omega(U_\Lambda) + \log \text{Tr}_A(e^{-\beta U_\Lambda}).
\] (24)

Taking \( \Lambda \to \infty \) for both sides of (24) and noting positivity of relative entropy we obtain

\[
0 \leq h(\omega \parallel \Phi, \beta) := \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} S(\omega_\Lambda|\rho^\text{IG}_\Lambda) = -s(\omega) + \beta e_{\Phi}(\omega) + P(\beta \Phi).
\] (25)

We shall call \( h(\omega \parallel \Phi, \beta) \) given in (25) the information rate of \( \omega \) with respect to \( \Phi \) at \( \beta \). (We refer to Eq.(15.32) of [25].) By substituting a translation invariant weak-\* accumulation point of \( \{\rho^\text{IG}_\Lambda, \Lambda \in \mathfrak{F}_{\text{loc}}\} \) into \( \omega \), the supremum of (22) is attained. Now we arrive at the general definition as follows.

**Definition 3 (Variational principle for translation invariant states)** A translation invariant state \( \varphi \) on \( \mathcal{A} \) is called a translation-invariant thermal equilibrium state for a translation covariant potential \( \Phi \) at \( \beta \), or shortly translation-invariant \((\Phi, \beta)\)-thermal equilibrium state, if

\[
h(\varphi \parallel \Phi, \beta) = 0.
\] (26)

Let \( \mathcal{S}_\gamma^{\text{Var}}(\Phi, \beta) \) denote the set of all translation-invariant \((\Phi, \beta)\)-thermal equilibrium states.

Now we comment on possible potentials for the above definitions. The existence of \( P(\Phi) \) and \( e_{\Phi}(\omega) \) can be verified if the translation covariant \( \Phi \) belongs to “the big Banach space of interactions” [20] satisfying that

\[
\sum_{\Lambda \neq 0} \frac{1}{|\Lambda|} ||\Phi(A)|| < \infty.
\] (27)

For such \( \Phi \), Definition 3 makes sense, but it is too broad. We need to require the existence of surface energies \( W_\Lambda \in \mathcal{A} \) for all \( \Lambda \in \mathfrak{F}_{\text{loc}} \) satisfying the asymptotic condition (10). (For example, if a translation covariant \( \Phi \) satisfying (27) has a finite-body interaction, namely \( \sup \{|\Lambda|; \Lambda \in \mathfrak{F}, \Phi(\Lambda) \neq 0\} < \infty \), then we have surface energies satisfying (10).) Furthermore, we need a strongly continuous one-parameter group of \( \ast \)-automorphisms \( \alpha_t \) (\( t \in \mathbb{R} \)) of \( \mathcal{A} \) as in (9). (We may refer to §6.2 of [8] and [26] for sufficient conditions of the existence of \( \alpha_t \) (\( t \in \mathbb{R} \)). But it should be emphasized that any particular decay condition of \( \Phi \) is not necessary.)
As the notations $S_{\text{KMS}}(\alpha_t, \beta)$, $S_{\text{Gibbs}}(\alpha, \Phi, \beta)$, and $S_{\text{Var}}(\Phi, \beta)$ indicate, the above definitions of thermal equilibrium depend on different elements. However, for the translation covariant $\Phi$ satisfying the set of assumptions stated in §2.2, the KMS condition, the AI Gibbs condition, and the variational principle are all equivalent for translation invariant states. We refer to Theorem 6.2.42 [8] and [21] for the details.

3 Variational Principle in Terms of Relative Entropy Density

Before we proceed to our result, let us reflect upon the variational principle and quantum relative entropy stated in the preceding section. Definition 3 uses $h(\omega || \Phi, \beta)$, a thermodynamic limit of quantum relative entropies per volume, where the first argument is the reduced states $\{\omega_A; A \in \mathcal{F}_{\text{loc}}\}$ of one global translation invariant state $\omega$, whereas the second argument is the set of internal canonical Gibbs states. Of course, $\{\rho^I_G; A \in \mathcal{F}_{\text{loc}}\}$ does not satisfy the consistency to determine a global state, a one-site interaction. This mismatch between the first and the second arguments of $h(\omega || \Phi, \beta)$ seems not comfortable, if we recall the entropy density $s(\omega)$ appeared in the variational principle; the entropy density is given by the thermodynamic limit of relative entropy densities $S(\omega_A | \text{tr}_A)$ for two translation invariant states $\omega$ and $\text{tr}$. Thus, from our aesthetic viewpoint, we like to use the relative entropy density for two translation invariant states in stead of $h(\omega || \Phi, \beta)$. This is done in the following theorem.

**Theorem 1** (Variational principle in terms of relative entropy density) Let $\beta$ be any positive constant. Let $\Phi$ be a translation covariant potential satisfying the conditions stated in §2.2. Let $\psi$ be any $(\Phi, \beta)$-translation invariant thermal equilibrium state. Then for any translation invariant state $\omega$

$$h(\omega | \psi) := \lim_{A \to \infty} \frac{1}{|A|} S(\omega_A | \psi_A)$$

exists in the van Hove limit, and the equality

$$h(\omega | \psi) = h(\omega || \Phi, \beta)$$

holds. (Hence the relative entropy density $h(\omega | \psi)$ expresses the free energy of the translation invariant state $\omega$ minus the uniquely determined free energy of the equilibrium up to the overall constant.)

A translation invariant state $\varphi$ attains

$$h(\varphi | \psi) = 0$$

if only if $\varphi$ is a $(\Phi, \beta)$-translation invariant thermal equilibrium state. Automatically such $\varphi$ satisfies the $(\alpha_t, \beta)$-KMS condition and the $(\Phi, \beta)$-AI Gibbs condition, where $\alpha_t$ is generated by $\Phi$.

**Proof** The proof we will present below faithfully follows the argument of [5]. First note that a thermal equilibrium state $\psi$ is an $(\alpha_t, \beta)$-KMS state [8]. So the von Neumann algebra $\mathcal{M}_\psi$ generated by the GNS representation $(\mathcal{H}_\psi, \pi_\psi, \Omega_\psi)$ of $\psi$ has a cyclic and separating vector $\Omega_\psi \in \mathcal{H}_\psi$. Due to [6] the perturbed vector (14) defined by the Dyson series in terms of (unbounded) modular operators can be written by bounded operators. (Note that [6] uses the notation $\beta = -1$. According to the authors, its basic idea comes from [22].) Hence
\( \Omega_\psi(\beta W_A) \) can be written as follows:

\[
\Omega_\psi(\beta W_A) = B(\beta W_A)\Omega_\psi, \quad B(\beta W_A) \equiv \theta \left( \pi_\psi \left( -\frac{1}{2} \beta W_A \right) \right) \in \mathfrak{M}_\psi \tag{31}
\]

where \( \theta(V) \in \mathfrak{M}_\psi \) for \( V \in \mathfrak{M}_{\psi,s} \) is explicitly given in §1 of [6]. By applying the argument of [28] (Theorem 12) to (31) we have

\[
\Omega_\psi(\beta W_A) = j_\psi(B(\beta W_A))\Omega_\psi, \tag{32}
\]

where \( j_\psi(R) = J_\psi R J_\psi \) for \( R \in \mathfrak{M}_\psi \), and \( J_\psi \) is the modular conjugation operator. Note that \( J_\psi \) is an antiunitary involution such that \( j_\psi(M_\psi) = M_\psi' \), and \( J_\psi \Omega_\psi(V) = \Omega_\psi(V) \) for any \( V \in \mathfrak{M}_{\psi,s} \) as shown in [28]. Then for any \( R \in \mathfrak{M}_\psi \)

\[
\psi^{\beta W_A}(R^* R) = \left( \Omega_\psi(\beta W_A), \ R^* R \Omega_\psi(\beta W_A) \right) = \left( j_\psi(B(\beta W_A))\Omega_\psi, \ R^* R j_\psi(B(\beta W_A))\Omega_\psi \right) = \left( R\Omega_\psi, \ j_\psi(B(\beta W_A)^* B(\beta W_A)) R\Omega_\psi \right) \leq \| j_\psi(B(\beta W_A)^* B(\beta W_A)) \| (R\Omega_\psi, \ R\Omega_\psi) = \| B(\beta W_A) \|^2 \psi(R^* R). \tag{33}
\]

By Lemma 7 of [6], we have the following estimate of bounded operators \( \{ B(\beta W_A) \in \mathfrak{M}_\psi : \ A \in \mathfrak{A}_{\text{loc}} \} \)

\[
\| B(\beta W_A) \| \leq \exp \left( \frac{1}{2} c \beta \| W_A \| \right). \tag{34}
\]

where \( c \) is some positive constant that does not depend on either \( \beta \) or \( W_A \). From (33) and (34) we have the following majorization

\[
\psi^{\beta W_A} \leq \exp(c \beta \| W_A \|) \psi. \tag{35}
\]

As \( \psi^{-h} = \psi \) for any \( h \in \mathfrak{A}_{\text{sa}} \), by repeating a similar argument we have also

\[
\psi \leq \exp(c \beta \| W_A \|) \psi^{\beta W_A}. \tag{36}
\]

By the Peierls–Bogolubov inequality and the Golden–Thompson inequality [29] we have

\[
\exp(\psi(\beta W_A)) \leq \psi^{\beta W_A}(1) \leq \psi(\exp(\beta W_A)), \tag{37}
\]

which yields

\[
\exp(-\beta \| W_A \|) \leq \psi^{\beta W_A}(1) \leq \exp(\beta \| W_A \|). \tag{38}
\]

From (35), (36), and (38) it follows that

\[
\exp(-(c + 1)\beta \| W_A \|) \psi \leq [\psi^{\beta W_A}] \leq \exp((c + 1)\beta \| W_A \|) \psi. \tag{39}
\]

Taking the state-restriction of (39) to \( A \), and noting \([\psi^{\beta W_A}]_A = \rho^\text{IG}_A \) due to (17) we have

\[
\exp(-(c + 1)\beta \| W_A \|) \psi_A \leq \rho^\text{IG}_A \leq \exp((c + 1)\beta \| W_A \|) \psi_A. \tag{40}
\]

Since the logarithm function \( \log t \) is known to be operator monotone [30], we have the following operator inequalities

\[
-(c + 1)\beta \| W_A \| \leq \log D(\rho^\text{IG}_A) - \log D(\psi_A) \leq (c + 1)\beta \| W_A \|. \tag{41}
\]
By (41) and the assumption (10) we have

\[ \lim_{\Lambda \to \infty} \frac{\| \log D (\rho^G_\Lambda) - \log D (\psi_\Lambda) \|}{|\Lambda|} = 0. \] (42)

By direct computation we have

\[ S(\omega_\Lambda | \rho^G_\Lambda) - S(\omega_\Lambda | \psi_\Lambda) = \omega_\Lambda \left( \log D (\psi_\Lambda) - \log D (\rho^G_\Lambda) \right). \] (43)

By combining (42) and (43) we have the identity (29) as

\[ \lim_{\Lambda \to \infty} \frac{|S(\omega_\Lambda | \rho^G_\Lambda) - S(\omega_\Lambda | \psi_\Lambda)|}{|\Lambda|} = 0. \] (44)

By this and Definition 3 a translation invariant state \( \psi \) is a thermal equilibrium state if only if \( h(\psi | \psi) = 0 \).

**Remark 2** Theorem 1 tells limitation of the relative entropy density to distinguish two translation invariant states. If some translation covariant inner group is spontaneously broken admitting distinct translation invariant thermal equilibrium states, say \( \psi_1 \) and \( \psi_2 \), then \( h(\psi_1 | \psi_2) = 0 = h(\psi_1 | \psi_2) \), even though they are disjoint states. One may also recall two translation invariant thermal equilibrium states that favor low entropy and low energy, respectively, as given in [31]. The relative entropy density of these two disjoint states vanishes.

**Remark 3** Viewing Theorem 1 one may compare the entropy density of a translation invariant thermal equilibrium state \( \psi \) with the mean entropy of \( \{ \rho^G_\Lambda : \Lambda \in \mathcal{F}_{\text{loc}} \} \). In general, these can be different due to first-order phase transitions [31]. A sufficient condition of the equality is given in [32].

The second theorem is concerned with McMillan type convergence of entropy operators of reduced density matrices for a factorial translation invariant thermal equilibrium state. The topological notion considered there is “almost uniform convergence of a sequence of operators in a von Neumann algebra” introduced in [33].

**Theorem 2** (McMillan type convergence Theorem) Let \( \Phi \) be a translation covariant potential satisfying the conditions stated in § 2.2. Let \( \psi \) be any factor translation invariant thermal equilibrium state. Then the convergence

\[ \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \pi_\psi (- \log D (\varphi_\Lambda)) = s(\psi) \] (45)

holds almost uniformly.

**Proof** Owing to (42) in Theorem 1 we can apply the same argument in [34] to derive (45). \( \square \)

### 4 Discussions

Theorem 1 was shown under the assumption that admits only unique thermal equilibrium state [5]. The same statement was noted recently in [35]. We also refer to [36] for some related topic. The argument given in [5] relies on the analyticity of \( \mathcal{A} \)-valued functions \( \alpha_t (A) \in \mathcal{A} \) of \( t \in \mathbb{R} \) for \( A \in \mathcal{A}_{\text{loc}} \). However, this analyticity can not hold for general quantum spin lattice models as shown in [37]. In this paper, removing such unnecessary restriction we establish a quantum version of the Föllmer’s classical result for a general class of potentials. The second theorem is concerned with McMillan type convergence of entropy operators of reduced density matrices for a factorial translation invariant thermal equilibrium state. The topological notion considered there is “almost uniform convergence of a sequence of operators in a von Neumann algebra” introduced in [33].

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**Proof** Owing to (42) in Theorem 1 we can apply the same argument in [34] to derive (45). \( \square \)
that admits multiple equilibrium states. In the literature, there are increasing number of works that apparently intend to consider general properties of thermal equilibrium states, but impose the unique phase assumption due to mainly technical reasons. So let us advocate: Go beyond the unique phase assumption if not essential. (One may recall [15] which generalized [14] avoiding the argument based on the analyticity.)

We address some related issues. In Theorem 1 the assumption (10) upon surface energies is essential. On the other hand, the variational principle as stated in Definition 3 does not even require the existence of surface energies (6). So it is interesting to check or disprove Theorem 1 for a long-range potential $\Phi$.

It is a straightforward task to extend Theorem 1 to fermion lattice systems [21]. However, the case for continuous quantum systems is not so easy, see [38]. It is worth mentioning that one can extend Theorem 1 to the case where the full translation symmetry is broken to the periodic one, see the argument of Prop.5.3.7 of [39].

The key estimate (41) is determined by the norm of surface energies, and it does not matter whether a thermal equilibrium state is a pure phase (factor state) or a mixture of multiple phases (non-factor state). For the latter, we speculate that some long-range effect appears in its reduced densities as suggested in [40].

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