Gibbs variational formula in terms of quantum relative entropy density

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Abstract We prove the Gibbs variational formula for quantum lattice systems in terms of quantum relative entropy density. 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

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1 Introduction

The Dobrushin-Lanford-Ruelle (DLR) condition [1] [2] is a corner stone of rigorous statistical mechanics. It precisely characterizes thermal equilibrium states based on probability theory, see e.g. [3]. In particular, translation invariant thermal equilibrium states are identified with those states satisfying the minimum-free energy condition. This is usually referred to as the Gibbs variational principle, and has been proved for classical lattice systems [4] and for quantum lattice systems [5].

Notably the Gibbs variational principle can be expressed in terms of the relative entropy (or Kullback-Leibler divergence [6]) as given in [7] for classical systems. In this note, we establish an analogous statement for quantum lattice systems. In more detail we will prove the following: For any translation covariant potential $\Phi$, 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 $h(\omega \parallel \psi)$ of $\omega$ with respect to any translation invariant thermal equilibrium state $\psi$ for $\Phi$. This equivalence yields the characterization of translation invariant thermal equilibrium states $\varphi$ by $h(\varphi \parallel \psi) = 0$.

Let us compare our results with the previous work [8] by Hiai-Petz. In [8] under a limited setup that admits only a unique thermal equilibrium state $\psi$, the equality

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\[ h(\omega | \Phi, \beta) = h(\omega | \psi) \] is verified. On the other hand, we prove this equality for a much wider class of potentials that may have multiple phases. Owing to this equality we can establish the variational principle for thermal equilibrium states for quantum lattice systems as in [7].

2 Preliminaries

In this section we give our formulation that is based on C*-algebraic quantum statistical physics [9] [10]. 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 due to Umegaki [11], a fundamental quantity of this paper. Consider any finite dimensional full matrix algebra \( M_n(C) \) \((n \in \mathbb{N})\). Let \( \text{Tr} \) denote the matrix trace which takes 1 on each one-dimensional projection. Let \( \psi_1 \) and \( \psi_2 \) be states on \( M_n(C) \) 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

\[
S(\psi_1 | \psi_2) = \begin{cases} \psi_1 \left( \log D(\psi_1) - \log D(\psi_2) \right) & \text{if } \text{supp} \psi_1 \leq \text{supp} \psi_2 \\ +\infty & \text{otherwise} \end{cases}
\]

It is a quantum analogue of Kullback-Leibler divergence [6]. Let \( \text{tr} \) be a tracial state on \( M_n(C) \), i.e., \( \text{tr} = \frac{1}{n} \text{Tr} \). Then for a state \( \psi \) on \( M_n(C) \) its von Neumann entropy \( S(\psi) \) is given in terms of the quantum relative entropy as

\[
S(\psi) \equiv \psi(- \log D(\psi)) = -S(\psi | \text{tr}) + \log n.
\]

2.2 Quantum lattice systems

We consider a quantum spin lattice system on a cubic lattice \( \mathbb{Z}^\nu \) of arbitrary dimension \( \nu \in \mathbb{N} \). For any subset \( \Lambda \subset \mathbb{Z}^\nu \) let \(|\Lambda|\) denote the number of sites in \( \Lambda \). \(|\Lambda|\) will be identified with the volume of \( \Lambda \). \( \Lambda \) is a finite subset of \( \mathbb{Z}^\nu \) with finite \(|\Lambda| < \infty \). Let \( \mathcal{F}_{\text{loc}} := \{ \Lambda : \Lambda \in \mathbb{Z}^\nu \} \), the set of all finite subsets of \( \mathbb{Z}^\nu \).

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

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

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

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

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

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 $\Lambda \in \mathcal{A}_{\text{loc}}$ is given as

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

(5)

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

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

(6)

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

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

(7)

For any $I \in \mathcal{A}_{\text{loc}}$, 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 $J \in \mathcal{A}_{\text{loc}}$ is any finite subset such that $J \supset I$. By the set of consistent equations (8) for all $I \in \mathcal{A}_{\text{loc}}$ we can uniquely determine $*$-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 $\alpha_t$ ($t \in \mathbb{R}$) determined by the translation covariant potential $\Phi$ denotes a quantum time evolution of the infinitely extended quantum system $\mathcal{A}$. Finally, we put the following crucial assumption:

$$\lim_{\Lambda \rightarrow \infty} \frac{\|W_\Lambda\|}{|\Lambda|} = 0.$$  

(10)

This asymptotic condition says that the ratio of the norm of the surface energy to the volume of the specified region will vanish in the thermodynamic limit.
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 \( \mathcal{A}(\Lambda) \):
\[
\omega_\Lambda(A) = \omega(A) \quad \forall A \in \mathcal{A}(\Lambda). \tag{11}
\]
For each \( \Lambda \in \mathcal{F}_{\text{loc}} \) the density matrix \( D_\Lambda \) for \( \omega \) is determined by
\[
\omega_\Lambda(A) = \text{Tr}_\Lambda(D_\Lambda A) \quad \forall A \in \mathcal{A}(\Lambda), \tag{12}
\]
where \( \text{Tr}_\Lambda \) denotes the matrix trace of \( \mathcal{A}(\Lambda) \). A state \( \omega \) on \( \mathcal{A} \) is translation invariant if
\[
\omega(\gamma_x(A)) = \omega(A) \quad \forall A \in \mathcal{A}, \forall x \in \mathbb{Z}^n. \tag{13}
\]
We denote the set of all states on \( \mathcal{A} \) by \( S(\mathcal{A}) \), and the set of all translation invariant states by \( S_\gamma(\mathcal{A}) \).

For any state \( \omega \) of \( \mathcal{A} \) the triplet \( (\mathcal{H}_\omega, \pi_\omega, \Omega_\omega) \) denotes its GNS representation \([9]\). 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 \( \pi_\omega \) denotes the commutant. We denote the commutant algebra by \( \mathcal{M}_\omega' := \{ X \in \mathcal{B}(\mathcal{H}_\omega); [X, R] = XR - RX = 0 \quad \forall R \in \mathcal{M}_\omega \} \) and the center by \( \mathcal{Z}_\omega := \mathcal{M}_\omega \cap \mathcal{M}_\omega' \). A state \( \omega \) is called a factor state if its center is trivial, i.e. \( \mathcal{Z}_\omega = C I \), where I denotes the identity operator in \( \mathcal{H}_\omega \). In physics, a factor state corresponds to a pure 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 \([12][13]\). There are several reasons to consider that the KMS condition is the most fundamental notion of thermal equilibrium for quantum systems among others, see \([10]\). As one can see from Definition \([1]\) below due to \([14]\), the KMS condition is essentially based on quantum time evolution, whereas the DLR condition is directly defined in terms of the potential (specification), see \([15]\) for these two conditions. Hence between the quantum system and the classical system, such a big difference about the description of thermal equilibrium lies. So it is not straightforward to extend the classical results by Föllmer \([7]\) to the quantum system.

**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 \( \mathring{D}_\beta \). 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:

For every \( A \) and \( B \) in \( \mathcal{A} \), there exists a complex function \( F_{A,B}(z) \) of \( z \in D_\beta \) such that
(1) $F_{A,B}(z)$ is analytic in $D_B$.
(2) $F_{A,B}(z)$ is continuous and bounded on $D_B$.
(3) For all $t \in \mathbb{R}$, $F_{A,B}(t) = \varphi(\Delta \alpha \beta(B))$, $F_{A,B}(t + i\beta) = \varphi(\alpha \beta(B) \Lambda)$.

The set of all $(\alpha \beta \cdot \text{KMS})$ states is denoted as $S_{\text{KMS}}(\alpha \beta \cdot \mathcal{A})$.

It is useful to review some consequences of the above KMS condition. Let $\varphi$ be a KMS state and $(\mathcal{M}_\varphi, \pi_\varphi, \Omega_\varphi)$ 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 $X = 0$. The cyclic and separating vector $\Omega_\varphi \in \mathcal{H}_\varphi$ is an essential requirement of Tomita-Takesaki modular theory [16], and let $\Delta_\varphi$ denote the modular operator for $(\mathcal{M}_\varphi, \Omega_\varphi)$. The state $\varphi$ on $\mathcal{M}_\varphi$ given by $\varphi(X) = \langle \Omega_\varphi, X \Omega_\varphi \rangle$ for $X \in \mathcal{M}$ satisfies the KMS condition for the modular automorphism group $\sigma_t := \text{Ad}(\Delta_\varphi) (t \in \mathbb{R})$ at the inverse temperature $\beta = -1$. (This minus sign of $\beta$ requires obvious change in Definition1)

With the above background of the KMS condition and Tomita-Takesaki theory at hand, we recall another characterization of thermal equilibrium due to Araki-Ion [17] [18]. We name this characterization the Araki-Ion quantum Gibbs condition, or shortly, the AI Gibbs condition. As the AI Gibbs condition rigorously defines “Gibbs states” for quantum systems, it is considered as a quantum DLR condition. In fact, the AI Gibbs condition is reduced to the DLR condition for classical interactions. Furthermore, its formulation is more akin to the DLR condition than the KMS condition, since both the AI Gibbs condition and the DLR condition explicitly make use of surface energies and canonical local Gibbs states determined by the potential. On the other hand, the AI Gibbs condition is quite different from the DLR condition, since the AI Gibbs condition is a genuine quantum notion based on quantum dynamics as described below, whereas there is no dynamical concept for the DLR condition.

Let $\varphi$ a (KMS) state with its cyclic and separating GNS vector $\Omega_\varphi \in \mathcal{H}_\varphi$. We will perturb the KMS state $\varphi$ by $V \in \mathcal{M}_\text{sa}$ in the GNS space. As in [19] define

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

$$= \sum_{m=0}^{\infty} \int_0^1 dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{m-1}} \Delta_\varphi V \Delta_\varphi^{m-1-t} V \cdots \Delta_\varphi t V \Omega_\varphi$$

$$= \exp \left( \int_0^1 \Delta_\varphi V \Delta_\varphi^{-1} dt \right) \Omega_\varphi,$$  \hspace{1cm} (14)

where the sum converges absolutely, and the notation $\exp$ [20] denotes the Dyson time-ordering expansion [21]. If $V = \pi_\varphi(h)$ for $h \in \mathcal{A}_\text{sa}$, we denote the perturbed vector simply by $\Omega_\varphi(h)$. Then we obtain the positive linear functional and the state on $\mathcal{A}$ generated by this perturbed vector as

$$\varphi^h(A) := \langle \Omega_\varphi(h), \pi_\varphi(A) \Omega_\varphi(h) \rangle \quad A \in \mathcal{A},$$

$$\varphi^h(A) := \frac{\langle \Omega_\varphi(h), \pi_\varphi(A) \Omega_\varphi(h) \rangle - \varphi^h(1)}{\varphi^h(1)} \quad A \in \mathcal{A}.$$  \hspace{1cm} (15)
The weak extensions of $\varphi^h$ and $[\varphi^h]$ to $\mathcal{M}_\varphi$ are denoted by the same notations.

**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 $(\mathcal{H}_\varphi, \pi_\varphi, \Omega_\varphi)$ denote its GNS triplet. $\varphi$ 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 $\beta W_\Lambda$ has the following special product form

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

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

$$\rho^{IG}_A(A) = \frac{\text{Tr}_\Lambda(Ae^{-\beta U_\Lambda})}{\text{Tr}_\Lambda(e^{-\beta U_\Lambda})}, \quad A \in \mathcal{A}(\Lambda).$$

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

**Remark 1** The AI Gibbs condition is valid for all Gibbs states $\varphi$ of the infinite system $\mathcal{A}$. $\varphi$ is not necessarily a pure thermodynamic phase; it can be a statistical mixture of different phases.

**Remark 2** 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. (In the monograph [10] the AI Gibbs condition is given in Definition 6.2.16. Bratteli-Robinson’s notation $\omega_\Lambda$ means our $\rho^{IG}_A$, not $\varphi|_{\mathcal{A}(\Lambda)}$.)

**Remark 3** Instead of the product formula (17) one may consider the following weaker one

$$[\varphi^{\beta W_\Lambda}](A) = \rho^{IG}_A(A), \quad A \in \mathcal{A}(\Lambda).$$

This condition, which may be called “the weak Gibbs condition” [8], suffices to show our main theorem. Nevertheless the weak Gibbs condition implies the product formula (17) for quantum spin systems [18], and also for quantum fermion systems (under some additional assumption) [22].

From now on we focus on the translation-invariant case, i.e. translation invariant states for a translation covariant potential $\Phi$. Following the standard treatment of statistical mechanics we prepare thermodynamic functions [10] [15]. We use the van Hove limit $\Lambda \to \infty$ for an appropriate notion of thermodynamic limit. The pressure is defined as the following thermodynamic limit:

$$P(\Phi) := \lim_{\Lambda \to \infty} \frac{1}{|A|} \log \text{Tr}_\Lambda(e^{-U_\Lambda}).$$

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

$$e_\Phi(\omega) := \lim_{\Lambda \to \infty} \frac{1}{|A|} \omega(U_\Lambda),$$
and the entropy density is given by

\[ s(\omega) \equiv \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} S(\omega|\Lambda). \] (22)

The strong subadditivity of quantum entropy [23] is known to imply 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:

\[ P(\beta \Phi) = \sup_{\omega \in S(\gamma)} \left\{ s(\omega) - \beta e_\Phi(\omega) \right\}. \] (23)

The quantity \( s(\omega) - \beta e_\Phi(\omega) \) in the right-hand side is the free energy of the state \( \omega \) multiplied by the constant \(-\beta\). The variational formula characterizes thermal equilibrium as the minimum free-energy condition [4]: A translation invariant state \( \varphi \) is called a thermal equilibrium state if it takes the supremum of (23):

\[ P(\beta \Phi) = s(\varphi) - \beta e_\Phi(\varphi). \] (24)

Let us briefly derive the variational principle (23) with the help of quantum relative entropy. First we note the following identity for any finite system on \( \Lambda \in \mathcal{F}_{\text{loc}} \):

\[ S(\omega|\rho^A_\Lambda) = -S(\omega|\Lambda) + \beta \omega(U_\Lambda) + \log \text{Tr}_\Lambda(e^{-\beta U_\Lambda}). \] (25)

Taking \( \Lambda \to \infty \) for both sides of (25) and noting positivity of relative entropy we obtain

\[ 0 \leq h(\omega \parallel \Phi, \beta) := \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} S(\omega|\rho^A_\Lambda) = -s(\omega) + \beta e_\Phi(\omega) + P(\beta \Phi). \] (26)

We shall call \( h(\omega \parallel \Phi, \beta) \) given in (26) the information rate of \( \omega \) with respect to \( \Phi \) at \( \beta \). (See Eq.(15.32) of [25].) By substituting a translation invariant weak-* accumulation point of \( \{\rho^A_\Lambda, \Lambda \in \mathcal{F}_{\text{loc}}\} \) into \( \omega \), the supremum of (23) is attained. Now we arrive at the following definition.

**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

\[ h(\varphi \parallel \Phi, \beta) = 0. \] (27)

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

Now we comment on possible potentials \( \Phi \). The existence of \( P(\Phi) \) and \( e_\Phi(\omega) \) can be verified when the translation covariant \( \Phi \) satisfies

\[ \sum_{A \geq 0} \frac{1}{|A|} \| \Phi(A) \| < \infty. \] (28)
The set of all such $\Phi$ forms so called “the big Banach space of interactions” [15]. If any translation covariant $\Phi$ satisfying the estimate (28) has a finite-body interaction, namely $\sup \{ |\Lambda| ; \Lambda \in \mathcal{F}, \Phi(\Lambda) \neq 0 \} < \infty$, then the surface energy $W_\Lambda$ exits for any $\Lambda \in \mathcal{F}_{\text{loc}}$ and the asymptotic condition (10) can be verified. Furthermore such $\Phi$ admits a strongly continuous one-parameter group of $^\ast$-automorphisms $\alpha_t$ ($t \in \mathbb{R}$) of $\mathcal{A}$ whose generator is $\delta_\Phi$ as in (9). See § 6.2 of [10] and [26] about the conditions of $\Phi$ that generates a strongly continuous $\alpha_t$ ($t \in \mathbb{R}$).

We then comment on relationship among the above characterizations of thermal equilibrium. Definitions 1, 2 and 3. As the notations $S_{\text{KMS}}(\alpha_t, \beta)$, $S_{\text{Gibbs}}(\alpha_t, \Phi, \beta)$ and $S_{\text{Var}}(\Phi, \beta)$ ($\mathcal{A}$) indicate, those depend on different elements; the KMS condition is given by $\alpha_t$, the variation principle is given by $\Phi$, whereas the AI Gibbs condition depends on both $\alpha_t$ and $\Phi$; the AI Gibbs condition is somewhat an intermediate notion. The KMS condition and the AI Gibbs condition do not necessitate the translation covariance $\mathcal{A}$ for $\Phi$. The equivalence of the KMS condition and the AI Gibbs condition follows from Tomita-Takesaki modular theory [19]. The variational principle $\Rightarrow$ the KMS condition can be shown for any translation covariant potential for which the thermodynamic functions and a strongly continuous one-parameter group of $^\ast$-automorphisms $\alpha_t$ ($t \in \mathbb{R}$) of $\mathcal{A}$ exist, see [27] and also [22]. To derive the AI Gibbs condition $\Rightarrow$ the variational principle, the extra assumption (10) of surface energies is essentially used in [18]. In summary, the KMS condition, the AI Gibbs condition, and the variational principle are equivalent for translation invariant states for a certain class of translation covariant potentials $\Phi$, see Theorem 6.2.42 [10] and [22]. In the following, a translation invariant state satisfying these equivalent conditions is termed a translation-invariant thermal equilibrium state. As noted before, we have at least one translation-invariant thermal equilibrium state by taking weak-$^\ast$ limit of internal canonical Gibbs states.

3 Variational principle in terms of relative entropy density

Before we proceed to our new results, let us reflect on the variational principle and quantum relative entropy. Definition 3 uses $h(\omega \parallel \Phi, \beta)$, a thermodynamic limit of quantum relative entropies per volume, where the first argument is the reduced states $\{ \omega_\Lambda ; \Lambda \in \mathcal{F}_{\text{loc}} \}$ of one global translation invariant state $\omega$, whereas the second argument is the set of internal canonical Gibbs states. Of course, $\{ \rho_\Lambda^{\text{IG}} ; \Lambda \in \mathcal{F}_{\text{loc}} \}$ does not satisfy $\rho_\Lambda^{(\Phi, \beta)} |_{\Lambda \subset J} = \rho_\Lambda^{(\Phi, \beta)} |_{\Lambda \subset I}$ for two finite subsets $J \supset I$ unless $\Phi$ is a trivial interaction. This mismatch between the first and the second arguments 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 $\frac{S(\omega_\Lambda | \rho_{\Lambda A}^{\text{IG}})}{|A|}$ for two translation invariant states $\omega$ and $\rho_{\Lambda A}^{\text{IG}}$ (with some trivial adjustment). For conceptual argument on “the usual Gibbs ansatz based on finite-box procedure versus the KMS condition based on the infinitely-extended C*-system” we may refer to [28] that prompted our investigation. In our opinion, the quantity $h(\omega \parallel \Phi, \beta)$ is a mixture of these two distinct concepts. From the above somewhat aesthetic standpoint, we would like to use the relative entropy density for two translation invariant
states on the infinitely-extended C*-system $\mathcal{A}$ 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 real number. 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 $\omega$

$$h(\omega \mid \psi) := \lim_{A \to \infty} \frac{1}{|A|} S(\omega_{A} \mid \psi_{A})$$

exists in the van Hove limit, and the equality

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

holds. A translation invariant state $\varphi$ attains

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

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** First note that a thermal equilibrium state $\psi$ is an $(\alpha_{t}, \beta)$-KMS state [10]. 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 [29] the perturbed vector (14) defined by the Dyson series in terms of (unbounded) modular operators can be written by bounded operators. (Note that [29] uses the notation $\beta = -1$. According to the authors, its basic idea comes from [30].) Hence $\Omega_{\psi}(\beta W_{\Lambda})$ can be written as follows:

$$\Omega_{\psi}(\beta W_{\Lambda}) = B(\beta W_{\Lambda})\Omega_{\psi}, \quad B(\beta W_{\Lambda}) \equiv \theta(\pi_{\psi}\left(-\frac{1}{2}\beta W_{\Lambda}\right)) \in \mathcal{M}_{\psi}$$

(32)

where $\theta(V) \in \mathcal{M}_{\psi}$ for $V \in \mathcal{M}_{\psi}$ is explicitly given in §1 of [29]. By applying the argument of [31] (Theorem 12) to [32] we have

$$\Omega_{\psi}(\beta W_{\Lambda}) = j_{\psi}(B(\beta W_{\Lambda}))\Omega_{\psi},$$

(33)

where $j_{\psi}(R) = J_{\psi}RJ_{\psi}$ for $R \in \mathcal{M}_{\psi}$, and $J_{\psi}$ is the modular conjugation operator. Note that $J_{\psi}$ is an antiunitary involution such that $j_{\psi}(\mathcal{M}_{\psi}) = \mathcal{M}_{\psi}$, and $J_{\psi}\Omega_{\psi}(V) = \Omega_{\psi}(V)$ for any $V \in \mathcal{M}_{\psi}$ as shown in [31]. Then for any $R$ in $\mathcal{M}_{\psi}$

$$\psi^{W_{\Lambda}}(R^{*}R) = \left(\Omega_{\psi}(\beta W_{\Lambda}), R^{*}R\Omega_{\psi}(\beta W_{\Lambda})\right)$$

$$= \left(\psi(B(\beta W_{\Lambda})), R^{*}R\psi(B(\beta W_{\Lambda}))\right) = \left(R\Omega_{\psi}, \psi(B(\beta W_{\Lambda})^{*}B(\beta W_{\Lambda}))R\Omega_{\psi}\right)$$

$$\leq \|\psi(B(\beta W_{\Lambda})^{*}B(\beta W_{\Lambda}))\| \left(R\Omega_{\psi}, R\Omega_{\psi}\right) = \|B(\beta W_{\Lambda})\|^{2}\psi(R^{*}R).$$

(34)
By Lemma 7 of [29], we have the following estimate of bounded operators \( \{B(\beta W_\Lambda) \in M_\psi : \Lambda \in \mathcal{F}_\infty \} \)

\[
\|B(\beta W_\Lambda)\| \leq \exp\left(\frac{1}{2}c\beta \|W_\Lambda\|\right),
\]

(35)

where \(c\) is some positive constant that does not depend on either \(\beta\) or \(W_\Lambda\). From (34) and (35) we have the following majorization

\[
\psi^{\beta W_\Lambda} \leq \exp(\psi^{\beta W_\Lambda}(1)) \psi^{\beta W_\Lambda}. \tag{36}
\]

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

\[
\psi \leq \exp(c\beta \|W_\Lambda\|) \psi^{\beta W_\Lambda}. \tag{37}
\]

By the Peierls-Bogolubov inequality and the Golden-Thompson inequality [32] we have

\[
\exp(\psi(\beta W_\Lambda)) \leq \psi^{\beta W_\Lambda}(1) \leq \psi(\exp(\beta W_\Lambda)), \tag{38}
\]

which yields

\[
\exp(-\beta \|W_\Lambda\|) \leq \psi^{\beta W_\Lambda}(1) \leq \exp(\beta \|W_\Lambda\|). \tag{39}
\]

From (36), (37), and (39) it follows that

\[
\exp(-(c+1)\beta \|W_\Lambda\|) \psi \leq [\psi^{\beta W_\Lambda}] \leq \exp((c+1)\beta \|W_\Lambda\|) \psi. \tag{40}
\]

Taking the state-restriction of (40) to \(\Lambda\), and noting \([\psi^{\beta W_\Lambda}]_\Lambda = \rho^{IG}_\Lambda\) due to (17) we have

\[
\exp(-(c+1)\beta \|W_\Lambda\|) \psi_\Lambda \leq \rho^{IG}_\Lambda \leq \exp((c+1)\beta \|W_\Lambda\|) \psi_\Lambda. \tag{41}
\]

Since the logarithm function \(\log t\) is known to be operator monotone [33], we have the following operator inequalities

\[
-(c+1)\beta \|W_\Lambda\| \leq \log D(\rho^{IG}_\Lambda) - \log D(\psi_\Lambda) \leq (c+1)\beta \|W_\Lambda\|. \tag{42}
\]

By (42) and the assumption (10) we have

\[
\lim_{\Lambda \to \infty} \frac{\|\log D(\rho^{IG}_\Lambda) - \log D(\psi_\Lambda)\|}{|\Lambda|} = 0. \tag{43}
\]

By direct computation we have

\[
S(\omega_\Lambda | \rho^{IG}_\Lambda) - S(\omega_\Lambda | \psi_\Lambda) = \omega_\Lambda \left(\log D(\psi_\Lambda) - \log D(\rho^{IG}_\Lambda)\right). \tag{44}
\]

By combining (42) and (44) we have the identity (30) as

\[
\lim_{\Lambda \to \infty} \frac{|S(\omega_\Lambda | \rho^{IG}_\Lambda) - S(\omega_\Lambda | \psi_\Lambda)|}{|\Lambda|} = 0. \tag{45}
\]

By this identity (30) and Definition 3, a translation invariant state \(\varphi\) is a thermal equilibrium state if only if \(h(\varphi | \psi) = 0\).
Remark 4 Viewing the above theorem, one may compare the entropy density of a translation invariant thermal equilibrium state $\varphi$ with the mean entropy of $\{\rho^\Lambda_G: \Lambda \in \Lambda_{\text{loc}}\}$. A sufficient condition of the equality of these two entropy densities is given in §14. However, in general, these can be different due to first-order phase transitions.

Our 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 §6.

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

$$\lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \pi_\varphi(-\log D(\varphi_\Lambda)) = s(\varphi)$$

(46)

holds almost uniformly.

**Proof** Owing to (43) in Theorem 1 we can apply the same argument in [37] to show (46).

4 Discussions

The same statement as Theorem 1 was shown for some limited case that admits only unique thermal equilibrium state [8]. Precisely the setup of [8] is finite-range potentials for one-dimensional quantum lattice system [38] or short-range potentials for a multi-dimensional quantum system at a sufficiently small $\beta > 0$ specified in Theorem 6.42 of [10]. The argument of [8] relies heavily on the analyticity of $\alpha_i$-valued functions $\alpha_i(A) \in \mathcal{A}$ of $i \in \mathbb{R}$ for $A \in \mathcal{A}_{\text{loc}}$. However, such analyticity can not be expected for general quantum spin lattice models as shown in [39]. It seems unsatisfactory to impose such a technical restrict upon the potential unless “the unique phase” is an essential demand for the statements. (In passing, we mention the work [40] that discusses general properties of thermal equilibrium states of quantum spin systems imposing the same strong restriction as in [8].)

In this work, by noting another perturbation formula of KMS states developed in [29] we obtain Theorem 1 and Theorem 2 under a more general setup that admits multiple thermal equilibrium states. In the course of proof, we make use the equivalent characterizations of thermal equilibrium, Definitions 1, 2 and 3.

We address some future problems. In Theorem 1 the assumption (10) upon surface energies is essential. On the other hand, the original formulation of the variational principle as stated in Definition 3 does not require this assumption (10) not even the existence of surface energies (6); it makes sense for a wider class of $\Phi$ satisfying the weaker decay condition (28). Presently we can not verify whether Theorem 1 is still valid for a long-range potential $\Phi$ that does not satisfy (10).
It is easy to extend Theorem 1 and Theorem 2 to fermion lattice systems [22]. We do not know whether similar results for continuous quantum systems are possible, c.f. [41].

Our key estimate (42) 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 unphysical state, we speculate that some long-range effect may manifest in its reduced densities as suggested in [42]. To see this we have to estimate non-local property of the bounded operator $B(\beta W_A)$ in (32) (35).

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