EQUILIBRIUM STATISTICAL MECHANICS FOR CLASSICAL AND QUANTUM UNBOUNDED SPIN SYSTEMS

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Abstract

We study the equilibrium statistical mechanics for classical and quantum unbounded spin systems interacting via superstable and regular interactions. We show that in classical systems any DLR measure satisfies the Gibbs variational equality and the converse is also true if the interaction is of finite range. For quantum systems, we show that the (weak) KMS state constructed via the thermodynamic limit of finite volume Green's functions satisfies the Gibbs variational equality.

Key words: Classical and quantum unbounded spin systems, superstable interaction, Gibbs (DLR) measures, KMS states, entropy, pressure, Gibbs variational principle.

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1. Introduction

In this paper we study the equilibrium statistical mechanics for classical and quantum unbounded spin systems. Mostly, we aim to show the equivalence of DLR equilibrium conditions and Gibbs variational equality (for classical systems) and to show that the (weak) KMS states satisfy the Gibbs variational equality (for quantum systems).

In bounded spin systems (that is, the single spin states correspond to compact sets and finite dimensional Hilbert spaces for classical and quantum systems, respectively) it has been well-established that the equilibrium states for the systems can be investigated via the tangent functionals to the pressure which is a convex function of interactions, or via the Gibbs variational principle, or via the DLR (resp. KMS) conditions, and these methods have turned out to be equivalent to each other (see the references [Is, Si2, Ge, BR2] and the original papers cited therein). So, it would be worthwhile to extend the theory to the unbounded systems. The study of unbounded (continuous) spin systems, which we consider in this paper, draws also much attention from its close connection with Euclidean quantum field theory [AH-K].

The interactions which we consider in this paper satisfy the superstability and regularity in the sense of Ruelle [R2]. The classical model for these interactions has been extensively investigated by Lebowitz and Presutti [LP]. In [LP], the existence of the thermodynamic limit of the pressure (free energy) for various boundary conditions has been proved. Moreover, the existence of equilibrium measures satisfying DLR conditions has been also shown in [LP]. We will show that the mean entropy for this system also exists and prove that any DLR measure satisfies the Gibbs variational equality and that the converse is also true if we further impose the finiteness of the interaction range. The quantum unbounded spin systems has been studied e.g., in [P1] aiming at the survey of the existence of the thermodynamic limit theory of pressure and the existence and uniqueness of the equilibrium states satisfying the (weak) KMS condition. In [PY], there has been proposed a characterization of Gibbs (equilibrium) states for quantum unbounded spin systems. In this paper, like in the classical case, we will show the existence of mean entropy and show that the (weak) KMS state constructed in [P1] via the thermodynamic limit of finite volume Green's functions satisfies the Gibbs variational principle.

We organize this paper as follows: In Section 2, we give necessary notations, preliminaries, and main results. The classical model is explained in Subsection 2.1 and the quantum model in Subseciton 2.2. In Section 3, we give the proofs for classical systems. Section 4 is devoted to the proof for quantum systems and in Appendix we prove some technical inequlities need in Section 4.

2. Notations, Preliminaries, and Main Results

2.1. Classical Systems

We consider the classical unbounded spin systems. Let $\mathbb{Z}^\nu$ be the ν-dimensional integer lattice. At each site $i \in \mathbb{Z}^\nu$, there corresponds a vector spin variable $s_i \in \mathbb{R}^d$. For $x := (x^1, \cdots, x^d) \in \mathbb{R}^d$ and $i := (i_1, \cdots, i_\nu) \in \mathbb{Z}^\nu$ we write

$$|x| := \Big[\sum_{l=1}^{d} (x^l)^2\Big]^{1/2}, \qquad |i| := \max_{1 \le l \le \nu} |i_\nu|.$$

When a subset $\Lambda \subset \mathbb{Z}^\nu$ is a finite set we will write $\Lambda \subset\subset \mathbb{Z}^\nu$. We will consider both interactions between the spins at different sites as well as self interactions. Throughout this paper we will impose the following conditions on the interaction:

Assumption 2.1. *The interaction $\Phi = (\Phi_\Delta)_{\Delta \subset\subset \mathbb{Z}^\nu}$ satisfies the following conditions:*

(a) Φ_Δ is a Borel measurable function on $(\mathbb{R}^d)^\Delta$ for each $\Delta \subset\subset \mathbb{Z}^\nu$.

(b) Φ_Δ is invariant under translations of $\mathbb{Z}^\nu$, i.e., for any $i \in \mathbb{Z}^\nu$, $\Phi_{\Delta+i} = \tau_i \Phi_\Delta$, where τ_i is the natural translation of functions.

(c) (Superstability) There are $A > 0$ and $c \in \mathbb{R}$ such that for every $x_\Lambda \in (\mathbb{R}^d)^\Lambda$,

$$V(x_\Lambda) := \sum_{\Delta \subset \Lambda} \Phi_\Delta(x_\Delta) \ge \sum_{i \in \Lambda} [A x_i^2 - c].$$

(d) (Strong regularity) There exists a decreasing positive function Ψ on the natural numbers such that

$$\Psi(r) \le K r^{-\nu-\varepsilon} \text{ for some } K \text{ and } \varepsilon > 0 \text{ with } \sum_{i \in \mathbb{Z}^\nu} \Psi(|i|) < A.$$

Furthermore, if Λ_1 and Λ_2 are disjoint finite subsets of $\mathbb{Z}^\nu$ and if one writes

$$V(x_{\Lambda_1 \cup \Lambda_2}) = V(x_{\Lambda_1}) + V(x_{\Lambda_2}) + W(x_{\Lambda_1}, x_{\Lambda_2})$$

then the bound

$$|W(x_{\Lambda_1}, x_{\Lambda_2})| \le \sum_{i \in \Lambda_1} \sum_{i \in \Lambda_2} \Psi(|i - j|) \frac{1}{2}(x_i^2 + x_j^2)$$

holds.

The Gibbs measures for the interaction Φ are defined on the configuration space $\Omega := (\mathbb{R}^d)^{\mathbb{Z}^\nu}$ in the following way. For each $\Lambda \subset \mathbb{Z}^\nu$ let $\pi_\Lambda : \Omega \to \Omega_\Lambda := (\mathbb{R}^d)^\Lambda$ be the projection, i.e., for $s := (s_i)_{i \in \mathbb{Z}^\nu} \in \Omega$, $\pi_\Lambda(s) := s_\Lambda := (s_i)_{i \in \Lambda} \in \Omega_\Lambda$. We let $\mathcal{F}_\Lambda^0$ denote the Borel σ-algebra on Ω_Λ and let $\mathcal{F}_\Lambda := \pi_\Lambda^{-1}(\mathcal{F}_\Lambda^0)$. We simply write $\mathcal{F}$ for $\mathcal{F}_{\mathbb{Z}^\nu}$. Denote by $\mathcal{P}(\Omega, \mathcal{F})$ the set of all probability measures on $(\Omega, \mathcal{F})$. We equip $\mathcal{P}(\Omega, \mathcal{F})$ with a topology, so called the topology of local convergence [Ge]: For each $\mu \in \mathcal{P}(\Omega, \mathcal{F})$ the sets

$$\{\nu \in \mathcal{P}(\Omega, \mathcal{F}) |\ \max_{1 \le k \le n} |\nu(A_k) - \mu(A_k)| < \varepsilon\}$$

with $A_1, \cdots, A_n \in \cup_{\Lambda \subset\subset \mathbb{Z}^\nu} \mathcal{F}_\Lambda$, $\varepsilon > 0$, and $n \geq 1$, form a base of neighborhoods of μ.

The following notion shall be useful throughout this paper.

Definition 2.2. *A probability measure μ on $(\Omega, \mathcal{F})$ is said to be regular if there exist $\overline{A} > 0$ and $\overline{\delta}$ so that for any $\Lambda \subset\subset \mathbb{Z}^\nu$, the projection μ_Λ of μ to $(\Omega, \mathcal{F}_\Lambda)$, which may be understood as a measure on $(\Omega_\Lambda, \mathcal{F}^0_\Lambda)$, is absolutely continuous with respect to $ds_\Lambda := \prod_{i\in\Lambda} ds_i$ with a Radon-Nikodym derivative $g(s_\Lambda|\mu)$ satisfying*

$$g(s_\Lambda|\mu) \leq \exp[-\sum_{i\in\Lambda}(\overline{A}s_i^2 - \overline{\delta})].$$

Before giving a definition of Gibbs measures we need to confine "possible confingurations". Let us define

$$\begin{aligned} \mathcal{S} &:= \cup_{N\in\mathbb{N}} \mathcal{S}_N, \\ \mathcal{S}_N &:= \{s \in \Omega | \forall\, l, \sum_{|i|\leq l} s_i^2 \leq N^2(2l+1)^\nu\}. \end{aligned} \tag{2.1}$$

It is easy to show that any regular measure is supported on $\mathcal{S}$. If $\mu \in \mathcal{P}(\Omega, \mathcal{F})$ satisfies $\mu(\mathcal{S}) = 1$, we say that μ is *tempered.*

The partition function in $\Lambda \subset\subset \mathbb{Z}^\nu$ for the interaction Φ with boundary condition $\overline{s} \in \mathcal{S}$ is defined by

$$Z^\Phi_\Lambda(\overline{s}) := \int ds_\Lambda \exp[-V(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})], \tag{2.2}$$

where $ds_\Lambda := \prod_{i\in\Lambda} ds_i$ and ds_i means the Lebesgue measure on $\mathbb{R}^d$ for each $i \in \mathbb{Z}^\nu$. The Gibbs specification $\gamma^\Phi = (\gamma^\Phi_\Lambda)_{\Lambda\subset\subset\mathbb{Z}^\nu}$ with respect to $\mathcal{S}$ is defined by [Ge, Pr]:

$$\gamma^\Phi_\Lambda(A|\overline{s}) := \begin{cases} \dfrac{1}{Z^\Phi_\Lambda(\overline{s})} \displaystyle\int ds_\Lambda \exp[-V(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})]\, 1_A(s_\Lambda \overline{s}_{\Lambda^c}), & \text{if } \overline{s} \in \mathcal{S} \\ 0, \quad \text{if } \overline{s} \notin \mathcal{S}, \end{cases} \tag{2.3}$$

where $A \in \mathcal{F}$ and 1_A is the indicator function on A and $s_\Lambda \overline{s}_{\Lambda^c} \in \Omega$ coincides with s_Λ on Λ and with $\overline{s}_{\Lambda^c}$ on Λ^c. It is easy to check that the Gibbs specification satisfies the consistency condition [Ge, Pr]: For $\Delta \subset \Lambda$, $\overline{s} \in \mathcal{S}$,

$$\begin{aligned} \gamma^\Phi_\Lambda \gamma^\Phi_\Delta(A|\overline{s}) &:= \int_{\mathcal{S}} \gamma^\Phi_\Lambda(ds'|\overline{s}) \gamma^\Phi_\Delta(A|s') \\ &= \gamma^\Phi_\Lambda(A|\overline{s}). \end{aligned} \tag{2.4}$$

The Gibbs measures are defined as follows [Ge, Pr, Si2]:

Definition 2.3. *A probability measure $\mu \in \mathcal{P}(\Omega, \mathcal{F})$ is said to be a Gibbs measure for the interaction Φ if μ is tempered and satisfies the following equilibrium equations (DLR conditions):*

$$\mu(A) = \int \mu(d\overline{s}) \gamma^\Phi_\Lambda(A|\overline{s}), \quad \Lambda \subset\subset \mathbb{Z}^\nu, \; A \in \mathcal{F}.$$

We denote by $\mathcal{G}(\Phi)$ the family of all Gibbs measures and by $\mathcal{G}^I(\Phi)$ the translationally invariant Gibbs measures.

For bounded functions f on Ω, we will sometimes use the notation

$$\gamma_\Lambda^\Phi(f|\overline{s}) := \int \gamma_\Lambda^\Phi(ds'|\overline{s}) f(s').$$

When Φ satisfies the conditions of Assumption 2.1, the existence of Gibbs measures was proven in [LP]:

Theorem 2.4. *([LP, Theorem 4.5]) Suppose that the interaction Φ satisfies the hypotheses of Assumption 2.1. Then, $\mathcal{G}(\Phi) \neq \emptyset$.*

We notice that $\mathcal{G}^I(\Phi)$ is also nonempty. In fact, for any $\mu \in \mathcal{G}(\Phi)$ and $i \in \mathbb{Z}^\nu$, it is easy to check that $\tau_i \mu \in \mathcal{G}(\Phi)$, where $\tau_i \mu$ is the translation of μ. So, any (weak*-)limit point of $\{\frac{1}{|\Lambda|}\sum_{i\in\Lambda}\tau_i\mu\}$ as Λ increases to $\mathbb{Z}^\nu$ belongs to $\mathcal{G}^I(\Phi)$ (see [Si2, Corollary III.2.10]).

The pressure, or the free energy, is defined in the following way. We consider the free boundary condition (b.c.), pure b.c., periodic b.c., and general b.c., respectively [LP]. The partition function in Λ with free b.c. is defined by

$$Z_\Lambda^\Phi := \int ds_\Lambda \exp[-V(s_\Lambda)] \tag{2.5}$$

and the (finite volume) pressure is defined by

$$P_\Lambda^\Phi := \frac{1}{|\Lambda|} \log Z_\Lambda^\Phi, \tag{2.6}$$

where $|\Lambda|$ means the volume (cardinality) of $\Lambda \subset\subset \mathbb{Z}^\nu$. In order to consider the pure b.c., for a technical reason, we need to introduce some subsets of Ω [LP]. For $a > 0$ let

$$X(a) := \{s \in \Omega |\, s_i^2 \le a \log |i|,\ \ |i| > 1\}. \tag{2.7}$$

For $\overline{s} \in X(a) \cap \mathcal{S}$, the partition function in the region $\Lambda \subset\subset \mathbb{Z}^\nu$ with pure b.c. $\overline{s}$ is given by the formula (2.2) and the pressure is defined by

$$P_\Lambda^\Phi(\overline{s}) := \frac{1}{|\Lambda|} \log Z_\Lambda^\Phi(\overline{s}). \tag{2.8}$$

Let us also define

$$\overline{X}(a) := \{s \in \Omega |\, \exists \Lambda(s) \subset\subset \mathbb{Z}^\nu,\ s_i^2 \le a \log |i| \text{ for } i \notin \Lambda(s)\}. \tag{2.9}$$

It is not hard to show that if $\nu \in \mathcal{P}(\Omega)$ is a regular measure, then for sufficiently large $a > 0$ we have

$$\nu(\overline{X}(a)) = 1. \tag{2.10}$$

Now, let $\nu \in \mathcal{P}(\Omega)$ be a regular measure. The finite volume pressure for the general b.c. ν is defined by

$$P_\Lambda^\Phi(\nu) := \int \nu(d\overline{s}) P_\Lambda^\Phi(\overline{s}). \tag{2.11}$$

Finally, we introduce the periodic b.c.. Consider the "torus" $T_n := (\mathbb{Z}/n\mathbb{Z})^\nu$ with the quotient map $q_n : \mathbb{Z}^\nu \to T_n$. The configuration space for T_n is $\Omega_{T_n} := (\mathbb{R}^d)^{T_n}$, and q_n induces a map $r_n : \Omega_{T_n} \to \Omega$ (repeating the configuration across $\mathbb{Z}^\nu$ with period n in each coordinate direction). The Hamiltonian for T_n is defined by [Is]

$$ {}_PH^\Phi_{T_n} := \sum_{[\Delta]}^{*} \Phi_\Delta \circ r_n, \tag{2.12} $$

where $[\Delta] := \{\Delta + nj \,|\, j \in \mathbb{Z}^\nu\}$ is the equivalence class and $\sum^{*}$ means that the sum is restricted to those Δ on which q_n is one-to-one. The pressure with periodic b.c. is defined by

$$ {}_PP^\Phi_{T_n} := n^{-\nu} \log \int_{T_n} ds_{T_n} \exp[-{}_PH^\Phi_{T_n}(s_{T_n})]. \tag{2.13} $$

The thermodynamic limit of the pressure for any b.c. is proved in [LP]. Recall that a sequence $\{\Lambda_n\}$, $\Lambda_n \subset\subset \mathbb{Z}^\nu$, is said to be tending to $\mathbb{Z}^\nu$ in the sense of van Hove (we write $\lim_{\Lambda_n \to \mathbb{Z}^\nu \text{ (van Hove)}}$ hereafter) if: (a) $\Lambda_{n+1} \supset \Lambda_n$, (b) $\Lambda_n \supset \Delta$ for any $\Delta \subset\subset \mathbb{Z}^\nu$ and some n, (c) given any parallelepiped Γ and the partition $\pi(\Gamma)$ of $\mathbb{Z}^\nu$ generated by translations of Γ

$$ \lim N^-_\Gamma(\Lambda_n) = \infty, \quad \lim \frac{N^-_\Gamma(\Lambda_n)}{N^+_\Gamma(\Lambda_n)} = 1, $$

where $N^-_\Gamma(\Lambda_n)$ is the number of sets of $\pi(\Gamma)$ contained in Λ_n, $N^+_\Gamma(\Lambda_n)$ the number of sets with non-void intersection with Λ_n.

Theorem 2.5. *([LP, Theorem 3.1]) Suppose that the hypotheses of Assumption 2.1 are satisfied and $\Lambda_n \to \mathbb{Z}^\nu$ in the sense of van Hove. Then, $\{P^\Phi_{\Lambda_n}\}$, $\{P^\Phi_{\Lambda_n}(\overline{s})\}$, and $\{P^\Phi_{\Lambda_n}(\nu)\}$ have the same thermodynamic limit, say P^Φ. Also, for the sequence of toruses $\{T_n\}$, the sequence $\{{}_PP^\Phi_{T_n}\}$ converges to the same limit P^Φ.*

We remark here that we have taken the definition for periodic b.c. from [Is], which differs slightly from that of [LP]. Still, it is not hard to see that the result of [LP] (for periodic b.c.) insists on to hold.

We now define the mean entropy for Gibbs measures. Let $\mu \in \mathcal{G}(\Phi)$ and suppose that f is a bounded $\mathcal{F}_\Lambda$-measurable function for some $\Lambda \subset\subset \mathbb{Z}^\nu$. By Gibbs condition we see that (we omit the superscript Φ in the notations if it involves no confusion)

$$ \begin{aligned} \mu(f) &= \int d\mu(\overline{s}) \gamma_\Lambda(f|\overline{s}) \\ &= \int ds_\Lambda f(s_\Lambda) \int d\mu(\overline{s}) \frac{1}{Z_\Lambda(\overline{s})} \exp[-V(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})] \\ &=: \int ds_\Lambda f(s_\Lambda) \mu^{(\Lambda)}(s_\Lambda). \end{aligned} \tag{2.14} $$

Thus, the restriction μ_Λ of μ to $\mathcal{F}_\Lambda$, which we may understand as a measure on Ω_Λ, is absolutely continuous w.r.t. ds_Λ with a Radon-Nikodym derivative $\mu^{(\Lambda)}(s_\Lambda)$,

$$\mu^{(\Lambda)}(s_\Lambda) = \int d\mu(\overline{s}) \frac{1}{Z_\Lambda(\overline{s})} \exp[-V(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})]. \tag{2.15}$$

The entropy of μ in $\Lambda \subset\subset \mathbb{Z}^\nu$ is defined by [Is, Si2]

$$S_\Lambda(\mu) := -\int ds_\Lambda \mu^{(\Lambda)}(s_\Lambda) \log \mu^{(\Lambda)}(s_\Lambda) = -\mu(\log \mu^{(\Lambda)}). \tag{2.16}$$

We will show that the mean entropy

$$s(\mu) := \lim_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} |\Lambda|^{-1} S_\Lambda(\mu) \tag{2.17}$$

exists. Furthermore, we will show that $\lim_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} |\Lambda|^{-1}\mu(H_\Lambda^\Phi)$, the limit of mean energy per unit volume, also exists and we have the Gibbs variational principle, which we state as a theorem:

Theorem 2.6. *Suppose that the interaction Φ satisfies the conditions of Assumption 2.1 and let $\mu \in \mathcal{G}^I(\Phi)$. Then, the mean entropy $s(\mu)$ and $\lim_{\Lambda \to \mathbb{Z}^\nu \textit{ (van Hove)}} |\Lambda|^{-1}\mu(H_\Lambda^\Phi)$ exist and satisfies the variational equality:*

$$s(\mu) - \lim_{\Lambda \to \mathbb{Z}^\nu \textit{ (van Hove)}} |\Lambda|^{-1}\mu(H_\Lambda^\Phi) = P^\Phi. \tag{2.18}$$

The proof of Theorem 2.6 will be given in the next section.

As in the case of bounded spin systems, the converse of Theorem 2.6 also holds. However, for a technical reason in the proof, we impose a further condition of finiteness of interaction range.

Theorem 2.7. *Suppose that a finite range interaction Φ satisfies the conditions of Assumption 2.1. Let $\mu \in \mathcal{P}(\Omega)$ be a translationally invariant regular measure (see Definition 2.2) and suppose that the variational equality (2.18) holds. Then $\mu \in \mathcal{G}^I(\Phi)$.*

The proof will be given in the next section.

2.2. Quantum Systems

Let us now turn our attention to the quantum systems. It is generally accepted that in quantum statistical mechanics the equilibrium states are those of KMS states [BR1-2, Is, Si2]. For quantum unbounded spin systems, by using the Green's function method [BR2], a state satisfying (weak) KMS condition has been constructed in [P1]. In [PY], there has been proposed a characterization of Gibbs states by using the concept of Gibbs measures and the conditional reduced density matrices. We will show that the (weak) KMS state constructed in [P1] satisfies the Gibbs variational equality. Let us begin with presenting necessary notations. We refer to [PY] for details.

For each bounded region $\Lambda \subset\subset \mathbb{Z}^\nu$ the Hilbert space for the unbounded spin systems is given by

$$\begin{aligned} \mathcal{H}_\Lambda &:= \otimes_{i\in\Lambda} L^2(\mathbb{R}^d, dx_i) \\ &= L^2((\mathbb{R}^d)^\Lambda, dx_\Lambda). \end{aligned} \tag{2.19}$$

The Hamiltonian operator for the region $\Lambda \subset\subset \mathbb{Z}^\nu$ is given by

$$H_\Lambda := -\frac{1}{2}\sum_{i\in\Lambda} \Delta_i + V(x_\Lambda), \tag{2.20}$$

where Δ_i is the Laplacian operator for the variable $x_i \in \mathbb{R}^d$ and $V(x_\Lambda)$ is the potential energy in the region Λ. We assume that the interaction Φ satisfies the hypotheses of Assumption 2.1.

For each bounded region $\Lambda \subset\subset \mathbb{Z}^\nu$, the C^*-algebra for local observables is defined by

$$\mathcal{A}_\Lambda := \mathcal{L}(\mathcal{H}_\Lambda), \tag{2.21}$$

where $\mathcal{L}(\mathcal{H}_\Lambda)$ is the algebra of all bounded operators on $\mathcal{H}_\Lambda$. If $\Lambda_1 \cap \Lambda_2 = \emptyset$, then $\mathcal{H}_{\Lambda_1\cup\Lambda_2} = \mathcal{H}_{\Lambda_1} \otimes \mathcal{H}_{\Lambda_2}$ and $\mathcal{A}_{\Lambda_1}$ is isomorphic to the C^*-algebra $\mathcal{A}_{\Lambda_1} \otimes \mathbf{1}_{\Lambda_2}$, where $\mathbf{1}_{\Lambda_2}$ denotes the identity operator on $\mathcal{H}_{\Lambda_2}$. In this way we identify $\mathcal{A}_\Lambda$ as a sub-algebra of $\mathcal{A}_{\Lambda'}$ when $\Lambda \subset \Lambda'$. Let

$$\mathcal{A} := \overline{\cup_{\Lambda\subset\subset\mathbb{Z}^\nu} \mathcal{A}_\Lambda} \tag{2.22}$$

be the C^*-algebra of the quasilocal observables. Notice that $\mathcal{A}$ has an identity.

The partition function in a region $\Lambda \subset\subset \mathbb{Z}^\nu$ is given by

$$Z_\Lambda^\Phi := \mathrm{Tr}_\Lambda(e^{-H_\Lambda}), \tag{2.23}$$

where Tr_Λ means the trace on the Hilbert space $\mathcal{H}_\Lambda$. Notice that by the superstability condition of Assumption 2.1 (c), e^{-H_Λ} belongs to the trace class and so Z_Λ^Φ is well defined as a finite number. The finite volume pressure is defined by

$$P_\Lambda^\Phi := \frac{1}{|\Lambda|} \log Z_\Lambda^\Phi. \tag{2.24}$$

We will again suppress the superscript Φ from the notations.

We notice that by the Feynman-Kac formula [Si1], the operator e^{-H_Λ} has its integral kernel function

$$e^{-H_\Lambda}(x_\Lambda, y_\Lambda) = \int P_{x_\Lambda,y_\Lambda}(ds_\Lambda) \exp\big[-\int_0^1 V(s_\Lambda(\tau))\, d\tau\big], \tag{2.25}$$

where x_Λ and y_Λ are points in $(\mathbb{R}^d)^\Lambda$, $s_\Lambda \in (C([0,1];\mathbb{R}^d))^\Lambda$, and $P_{x_\Lambda,y_\Lambda}(ds_\Lambda)$ is the conditional Wiener measure on the path space

$$\Omega_{x_\Lambda,y_\Lambda} := \{s_\Lambda \in (C([0,1];\mathbb{R}^d))^\Lambda |\, s_\Lambda(0) = x_\Lambda,\ s_\Lambda(1) = y_\Lambda\}.$$

(See e.g. [Si1] for details.) We will simply write $V(s_\Lambda)$ for $\int_0^1 V(s_\Lambda(\tau))\,d\tau$. Thus, the partition function Z_Λ can be rewritten as an integral over a path space:

$$Z_\Lambda = \int_{(\mathbb{R}^d)^\Lambda} dx_\Lambda \int_{\Omega_{x_\Lambda,x_\Lambda}} P_{x_\Lambda,x_\Lambda}(ds_\Lambda) e^{-V(s_\Lambda)}. \tag{2.26}$$

Since, by a translation $y_\Lambda \mapsto y_\Lambda - x_\Lambda$, the measure $P_{x_\Lambda,x_\Lambda}(ds_\Lambda)$ on $\Omega_{x_\Lambda,x_\Lambda}$ becomes the measure $P_{0,0}(ds_\Lambda) =: P(ds_\Lambda)$ on $\Omega_{0,0}$, by letting $\lambda(ds_\Lambda) := dx_\Lambda P(ds_\Lambda)$ on $(\mathbb{R}^d)^\Lambda \times \Omega_{0,0}$, the expression in (2.26) can be further simplified:

$$Z_\Lambda = \int \lambda(ds_\Lambda) e^{-V(s_\Lambda)}. \tag{2.27}$$

By using the above Wiener integral formalism and Ruelle-type probability estimates, Park has shown the existence of the thermodynamic limit of the pressure [P1]. We remark here that by introducing the concept of "Gibbs specifications" (and hence Gibbs measures) for quantum spin systems as in [PY], we can also define the finite volume pressures with different kind of boundary conditions like in the classical case (see (2.6), (2.8), and (2.11)). By extending the method of [LP] to the quantum case we can also prove that the thermodynamic limits of the pressure with different b.c. are the same (cf. Theorem 2.5). We need, however, only the result for the free b.c., which we state as a Theorem.

Theorem 2.8. *([P1, Theorem 2.2]) Suppose that the hypotheses of Assumption 2.1 hold. Then, the limit*

$$\lim_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} P_\Lambda^\Phi = P^\Phi$$

exits.

We now consider the equilibrium states for quantum systems. Define the finite volume Green's functions [BR2] by

$$G_\Lambda(A, B; t) := \omega_\Lambda(A\alpha_t^\Lambda(B)), \quad A,\ B \in \mathcal{A}_\Lambda, \tag{2.28}$$

where ω_Λ is the local Gibbs state on $\mathcal{A}_\Lambda$:

$$\omega_\Lambda(A) := \frac{1}{Z_\Lambda}\mathrm{Tr}_\Lambda(e^{-H_\Lambda}A), \quad A \in \mathcal{A}_\Lambda, \tag{2.29}$$

and α_t^Λ is the time evolution automorphism on $\mathcal{A}_\Lambda$:

$$\alpha_t^\Lambda(B) := e^{itH_\Lambda}Be^{-itH_\Lambda}, \quad B \in \mathcal{A}_\Lambda. \tag{2.30}$$

By Hahn-Banach theorem the state ω_Λ can be extended to a state on $\mathcal{A}$ and we use the same notation for the extension. Notice that G_Λ is bounded as

$$|G_\Lambda(A, B; t)| \le \|A\|\,\|B\|. \tag{2.31}$$

Thus by Tychonoff's theorem, there exists a subnet $\{\Lambda_n\} \subset \mathbb{Z}^\nu$ such that

$$G_\Lambda(A, B; t) := \lim_{n\to\infty} G_{\Lambda_n}(A, B; t) \tag{2.32}$$

exists for all $A,\ B \in \mathcal{A},\ t \in \mathbb{R}$ [BR2]. Clearly, the values

$$\omega(A) := G(A, B; t), \quad A \in \mathcal{A}, \tag{2.33}$$

determine a state ω over the quasilocal algebra $\mathcal{A}$. That is, ω is a positive-definite linear functional with norm one on $\mathcal{A}$. Let us impose a further condition on the interaction:

Assumption 2.9. *(Polynomial boundedness of interaction) There exist a constant $D > 0$ and a natural number n such that the one-body interaction $\Phi_{\{i\}}(x_i) \equiv P(x_i)$ satisfies the following bound:*

$$P(x_i) \le D(|x_i|^{2n} + 1), \quad i \in \mathbb{Z}^\nu.$$

Under the conditions of Assumption 2.1 and Assumption 2.9, Park has shown that the state ω in (2.33) satisfies a (weak) KMS condition. We refer to [P1] for the details. We take the state ω as a probe for our purpose.

The mean entropy for the states of quantum systems is defined as follows. Let ρ be any state on $\mathcal{A}$ and ρ_Λ the restriction of ρ to $\mathcal{A}_\Lambda$, $\Lambda \subset\subset \mathbb{Z}^\nu$. Suppose that ρ_Λ is a normal state on $\mathcal{A}_\Lambda$, i.e., there exists a density matrix $\rho^{(\Lambda)} \in \mathcal{A}_\Lambda$ such that

$$\rho_\Lambda(A) = \mathrm{Tr}_\Lambda(\rho^{(\Lambda)} A), \quad A \in \mathcal{A}_\Lambda. \tag{2.34}$$

The entropy of ρ in Λ is defined by [BR2, Is, Si2]

$$\begin{aligned} S_\Lambda(\rho) &:= -\mathrm{Tr}_\Lambda(\rho^{(\Lambda)} \log \rho^{(\Lambda)}) \\ &= -\rho_\Lambda(\log \rho^{(\Lambda)}). \end{aligned} \tag{2.35}$$

From the definition, we see that (we omit Φ from the notations)

$$S_\Lambda(\omega_\Lambda) - \omega_\Lambda(H_\Lambda) = |\Lambda| P_\Lambda. \tag{2.36}$$

In general we have the following properties:

Proposition 2.10. *Suppose that ρ is a state on $\mathcal{A}$ such that the restriction ρ_Λ of ρ to any $\mathcal{A}_\Lambda$, $\Lambda \subset\subset \mathbb{Z}^\nu$, is a normal state. Then, the following properties hold:*

(a) For any $\Lambda \subset\subset \mathbb{Z}^\nu$,

$$S_\Lambda(\rho) - \rho(H_\Lambda) \le |\Lambda| P_\Lambda. \tag{2.37}$$

(b) The mean entropy

$$s(\rho) := \lim_{a\to\infty} a^{-\nu} S_{C_a}(\rho) \tag{2.38}$$

exists, where C_a *is a cube of sides* a.

We will give a proof of Proposition 2.10 in Section 4. As a corollary to Proposition 2.10 we have the following variational inequality:

Corollary 2.11. *Suppose the hypotheses of Proposition 2.10 hold. Then, the inequality*

$$s(\rho) - \liminf_{a\to\infty} a^{-\nu}\rho(H_{C_a}) \le P^\Phi \tag{2.39}$$

holds.

One of the main purpose of this paper is to show that for the state ω given in (2.33) the equality holds in (2.39):

Theorem 2.12. *Suppose the hypotheses of Assumption 2.1 and 2.9 hold. Let* ω *be the equilibrium state given in (2.33). Then, the mean energy per unit volume* $\lim_{a\to\infty} a^{-\nu}\omega(H_{C_a})$ *exists and the equality*

$$s(\omega) - \lim_{a\to\infty} a^{-\nu}\omega(H_{C_a}) = P^\Phi$$

holds.

The proof of the above theorem will be given in Section 4.

3. Proofs of Main Results: Classical Systems

3.1. DLR measures satisfy the variational equality

In this subsection we will prove Theorem 2.6. Let $\mu \in \mathcal{G}(\Phi)$ be a Gibbs measure. Recall the definition of the entropy $S_\Lambda(\rho)$ in (2.16). We first give some properties of $S_\Lambda(\mu)$.

Lemma 3.1. *Let* $\mu \in \mathcal{G}(\Phi)$ *and* $S_\Lambda(\mu)$, $\Lambda \subset\subset \mathbb{Z}^\nu$, *be defined by (2.16). Then, the following properties hold:*

(a) $S_\Lambda(\mu) \le 0$ *(negativity).*

(b) $\Lambda \subset \Lambda' \Longrightarrow S_{\Lambda'}(\mu) \le S_\Lambda(\mu)$ *(decrease).*

(c) $S_{\Lambda\cup\Lambda'}(\mu) + S_{\Lambda\cap\Lambda'}(\mu) \le S_\Lambda(\mu) + S_{\Lambda'}(\mu)$ *(strong subadditivity).*

Proof. The proofs of (b) and (c) can be done by the same method given, e.g., in the proof of Lemma II.2.1 of [Is]. The property (a) will not be used in this paper, but we have given it as a property of the entropy. Since the a priori measure, the Lebesgue measure, is not a finite measure we can not simply take $S_\emptyset(\mu) \equiv 0$ as done in the proof of Lemma II.2.1 of [Is] for bounded spin systems. However, we can make a detour. Let us introduce a probability measure

$$d\mu^{(0)}(s_i) := N^{-1} \exp(-\alpha s_i^2) ds_i, \tag{3.1}$$

where $\alpha > 0$ is a sufficiently small number and $N := (\pi/\alpha)^{d/2}$ is the normalization constant. For each $\Lambda \subset\subset \mathbb{Z}^\nu$ let us define

$$\widetilde{V}(s_\Lambda) := V(s_\Lambda) - \sum_{i\in\Lambda} \alpha s_i^2. \tag{3.2}$$

We then have, by Gibbs condition, for $f \in L^1(\Omega; d\mu)$

$$\begin{aligned} \int f d\mu &= \int d\mu(\overline{s}) \frac{1}{Z_\Lambda(\overline{s})} \int ds_\Lambda \exp[-V(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})] f(s_\Lambda \overline{s}_{\Lambda^c}) \\ &= \int d\mu(\overline{s}) \frac{1}{Z_\Lambda^{(0)}(\overline{s})} \int d\mu^{(0)}(s_\Lambda) \exp[-\widetilde{V}(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})] f(s_\Lambda \overline{s}_{\Lambda^c}), \end{aligned} \tag{3.3}$$

where

$$Z_\Lambda^{(0)}(\overline{s}) := \int d\mu^{(0)}(s_\Lambda) \exp[-\widetilde{V}(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})] = N^{-|\Lambda|} Z_\Lambda(\overline{s}).$$

Let us define (see (2.15))

$$\begin{aligned} \mu_\Lambda^{(0)}(s_\Lambda) &:= \int d\mu(\overline{s}) \frac{1}{Z_\Lambda^{(0)}(\overline{s})} \exp[-\widetilde{V}(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})] \\ &= N^{|\Lambda|} \exp[\alpha \textstyle\sum_{i\in\Lambda} s_i^2]\, \mu^{(\Lambda)}(s_\Lambda). \end{aligned} \tag{3.4}$$

We notice that $\mu_\Lambda^{(0)}(s_\Lambda)$ is a Radon-Nikodym derivative of μ_Λ, the restriction of μ to $\mathcal{F}_\Lambda$, with respect to $\mu^{(0)}(\equiv (\mu^{(0)})^\Lambda)$. Define

$$S_\Lambda^{(0)}(\mu) := - < \mu_\Lambda^{(0)} \log \mu_\Lambda^{(0)} >^{(0)}, \tag{3.5}$$

where $< \cdot >^{(0)}$ is, obviously, the expectation w.r.t. $\mu^{(0)}$. Then, using (3.4) we have that

$$S_\Lambda(\mu) = |\Lambda|[\log N + a_0] + S_\Lambda^{(0)}(\mu), \tag{3.6}$$

where $a_0 := \alpha < s_i^2 >_\mu > 0$. By the usual method we have $S_\Lambda^{(0)}(\mu) \geq S_{\Lambda'}^{(0)}(\mu)$ for $\Lambda \subset \Lambda'$. Moreover, since $\mu^{(0)}$ is a probability measure, we may define $S_\emptyset^{(0)}(\mu) \equiv 0$. By putting $\Lambda = \emptyset$ in (3.6) we get $S_\emptyset(\mu) = 0$. Using the property (b) we obtain (a). ■

Proposition 3.2. *Suppose $\mu \in \mathcal{G}^I(\Phi)$. The mean entropy*

$$s(\mu) := \lim_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} |\Lambda|^{-1} S_\Lambda(\mu)$$

exists.

Proof. It follows from Lemma 3.1 and the same method given in [Is, Theorem II.2.2]. ∎

Proof of Theorem 2.6. Let us now suppose $\mu \in \mathcal{G}^I(\Phi)$. By Jensen's inequality we see that

$$\begin{aligned} S_\Lambda(\mu) - \mu(H_\Lambda) &= \mu(-\log \mu^{(\Lambda)} - H_\Lambda) \\ &\le \log \mu\left(\tfrac{e^{-H_\Lambda}}{\mu^{(\Lambda)}}\right) \\ &= \log < e^{-H_\Lambda} >_0 = |\Lambda| P_\Lambda, \end{aligned} \tag{3.7}$$

where $< \cdot >_0$ is the expectation with respect to the Lebesgue measure on Ω_Λ. Dividing both sides of (3.7) by $|\Lambda|$, taking limit supremum, and using Theorem 2.5 and Proposition 3.2, we get

$$s(\mu) - \liminf_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} \frac{1}{|\Lambda|}\mu(H_\Lambda) \le P^\Phi. \tag{3.8}$$

Next, for each $\Lambda \subset\subset \mathbb{Z}^\nu$ and $\overline{s} \in \mathcal{S} \cap \overline{X}(a)$ let us define a state $\mu_\Lambda^{(\overline{s})}$ on $C(\Omega_\Lambda)$ as follows: for any $f \in C(\Omega_\Lambda)$

$$\begin{aligned} \mu_\Lambda^{(\overline{s})}(f) &:= \frac{1}{Z_\Lambda(\overline{s})}\int ds_\Lambda \exp[-V(s_\Lambda) - W(s_\Lambda, \overline{s}_{\Lambda^c})] f(s_\Lambda) \\ &\equiv \int ds_\Lambda\, \mu^{(\Lambda|\overline{s})}(s_\Lambda) f(s_\Lambda). \end{aligned} \tag{3.9}$$

Notice that the function $0 \le t \mapsto g(t) := -t\log t$ is concave. Thus,

$$\begin{aligned} S_\Lambda(\mu) &= - < \mu^{(\Lambda)} \log \mu^{(\Lambda)} >_0 \\ &= < g(\textstyle\int d\mu(\overline{s})\mu^{(\Lambda|\overline{s})}) >_0 \\ &\ge -\int d\mu(\overline{s}) < \mu^{(\Lambda|\overline{s})} \log \mu^{(\Lambda|\overline{s})} >_0 \\ &= \int d\mu(\overline{s})\left[\log Z_\Lambda(\overline{s}) + \mu_\Lambda^{(\overline{s})}(V(\cdot) + W(\cdot, \overline{s}_{\Lambda^c}))\right] \\ &= |\Lambda| P_\Lambda(\mu) + \int d\mu(s)[H_\Lambda(s_\Lambda) + W(s_\Lambda, s_{\Lambda^c})], \end{aligned} \tag{3.10}$$

where we have used the notation (2.11) and the Gibbs condition to get the last equality. We assert that

$$\lim_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} \frac{1}{|\Lambda|}\int d\mu(s) W(s_\Lambda, s_{\Lambda^c}) = 0. \tag{3.11}$$

Under the condition of (3.11), after dividing both sides of (3.10) by $|\Lambda|$ and taking limsup, and using Theorem 2.5 and Proposition 3.2 again, we get

$$s(\mu) \ge P^\Phi + \limsup_{\Lambda \to \mathbb{Z}^\nu \text{ (van Hove)}} \frac{1}{|\Lambda|}\mu(H_\Lambda). \tag{3.12}$$

This, together with the inequality (3.8), completes the proof. So, it remains only to prove the assertion (3.11). In fact, by using the regularity of the interaction, monotone convergence theorem, and regularity of the Gibbs measure (see Definition 2.2) we see that

$$
\begin{aligned}
|\Lambda|^{-1}\int d\mu(s)|W(s_\Lambda, s_{\Lambda^c})| &\le |\Lambda|^{-1}\int d\mu(s)\sum_{i\in\Lambda}\sum_{j\in\Lambda^c}\Psi(|i-j|)\frac{1}{2}(s_i^2+s_j^2) \\
&\le c|\Lambda|^{-1}\sum_{i\in\Lambda}\sum_{j\in\Lambda^c}\Psi(|i-j|),
\end{aligned}
\tag{3.13}
$$

for some constant $c > 0$. Let us define for $r > 0$

$$\partial_r^-(\Lambda) := \{i \in \Lambda |\, \mathrm{dist}\,(i, \Lambda^c) \le r\}. \tag{3.14}$$

Notice that given $\varepsilon > 0$, there exists $r > 0$ such that

$$\sum_{j\in\mathbb{Z}^\nu:\,|j|\ge r}\Psi(|j|) \le \varepsilon. \tag{3.15}$$

We fix such a number $r > 0$. If Λ is sufficiently large, it is obvious that

$$|\Lambda|^{-1}|\partial_r^-(\Lambda)| \le \varepsilon. \tag{3.16}$$

Splitting the sum $\sum_{i\in\Lambda} = \sum_{i\in\Lambda\setminus\partial_r^-(\Lambda)} + \sum_{i\in\partial_r^-(\Lambda)}$ in (3.13) we see that the right hand side of (3.13) is bounded by $(c+J)\varepsilon$, where $J := \sum_{j\in\mathbb{Z}^n}\Psi(|j|)$. Since $\varepsilon > 0$ is arbitrary, this proves the assertion (3.11) and the proof of Thoerem 2.6 is now completed. ■

Remark 3.3. *When the interaction Φ is one-body and two-body interaction, i.e., $\Phi_\Delta = 0$ if $|D| \ge 3$, then one easily checks that the statement of Theorem 2.6 can be replaced by the usual form [Is, Si2]:*

$$s(\mu) - \mu(A_\Phi) = P^\Phi, \tag{3.16}$$

where $A_\Phi := \sum_{X\ni 0}\frac{1}{|X|}\Phi_X$.

3.2. Variational equality implies the DLR condition

In this subsection we will prove Theorem 2.7. We assume that the interaction Φ is of finite range, i.e., there exists $R > 0$ such that $\Phi_X = 0$ whenever $\mathrm{diam}(X) \ge R$, where $\mathrm{diam}(X) := \max\{|i-j|\,|\, i,j \in X\}$ is the diameter of X. Suppose that a translationally invariant measure $\mu \in \mathcal{P}(\Omega)$ is regular (see Definition 2.2) and satisfies the variational equality (2.18). We want to show that $\mu \in \mathcal{G}^I(\Phi)$. The key idea of the proof we have borrowed from that of Theorem III.2.1 of [Is].

Proof of Theorem 2.7. We have to show that for any bounded $\mathcal{F}$-measurable $f : \Omega \to \mathbb{R}$,

$$\mu(f - \gamma_\Lambda f) = 0, \quad \forall\, \Lambda \subset\subset \mathbb{Z}^\nu. \tag{3.17}$$

It is enough to show (3.17) only for local functions. So, suppose that f is $\mathcal{F}_{\Lambda'}$-measurable for some $\Lambda' \subset\subset \mathbb{Z}^\nu$. Let us put $F := f - \gamma_\Lambda f$. Since the interaction is of finite range F is also a local function, i.e., F is $\mathcal{F}_{\widetilde{\Lambda}}$-measurable for some finite $\widetilde{\Lambda} \supset \Lambda \cup \Lambda'$. Let us define an auxiliary interaction Ψ as follows:

$$\begin{cases} \Psi_{\widetilde{\Lambda}+i} = \tau_i F & \text{for } i \in \mathbb{Z}^\nu \\ \Psi_Y = 0 & \text{if } Y \text{ is not a translate of } \widetilde{\Lambda}. \end{cases} \tag{3.18}$$

Since Ψ is bounded and of finite range we see that the interaction $\Phi + \lambda\Psi$ is also superstable and regular for any $\lambda \in \mathbb{R}$. Recall the periodic boundary condition introduced in Subsection 2.1. Let $T_n := (\mathbb{Z}/n\mathbb{Z})^\nu$ be a sufficiently large torus so that $T_n \supset \widetilde{\Lambda}$. We let $< \cdot >_{n,\lambda}$ be the (local) Gibbs measure on T_n with pure b.c. for the interaction $\Phi + \lambda\Psi$, i.e.,

$$< A >_{n,\lambda} := \frac{1}{Z_{T_n}^{(\lambda)}} \int ds_{T_n} \exp[-{}_PH_{T_n}^{\Phi+\lambda\Psi}(s_{T_n})] A(s_{T_n}), \tag{3.19}$$

where the Hamiltonian ${}_PH_{T_n}^{\Phi+\lambda\Psi}$ is defined as in (2.12) and $Z_{T_n}^{(\lambda)}$ is the obvious normalizing factor. Given $\varepsilon > 0$ we claim that there exist $\lambda_0 > 0$ and $\mathcal{F}_{T_n}$-measurable functions $F^{(n,\lambda)}$, $|\lambda| \le \lambda_0$, such that

$$< F^{(n,\lambda)} >_{n,\lambda} = 0 \text{ and } \|F^{(n,\lambda)} - F\|_\infty \le \varepsilon. \tag{3.20}$$

In fact, for each $t \in \Omega_{T_n}$ (we regard T_n as a subset of $\mathbb{Z}^\nu$ if necessary) let us define

$$\gamma_\Lambda^{(n,\lambda)} f(t) := \frac{1}{Z_\Lambda^{(n,\lambda)}(t)} \int ds'_\Lambda \exp\Big[-{}_PH_{T_n}^{\Phi+\lambda\Psi}(s'_\Lambda t_{T_n\setminus\Lambda}) - \lambda \sum_{(i+\widetilde{\Lambda})\cap\Lambda\neq\emptyset} (\tau_i F)(s'_\Lambda t_{T_n\setminus\Lambda})\Big] f(s'_\Lambda t_{T_n\setminus\Lambda}), \tag{3.21}$$

where $Z_\Lambda^{(n,\lambda)}(t)$ is a normalization factor. We define

$$F^{(n,\lambda)}(t) := f(t) - \gamma_\Lambda^{(n,\lambda)} f(t), \quad t \in \Omega_{T_n}. \tag{3.22}$$

It is not hard to show that

$$< F^{(n,\lambda)} >_{n,\lambda} = 0. \tag{3.23}$$

In order to show that $\|F^{(n,\lambda)} - F\|_\infty \le \varepsilon$, without loss, we may assume $f \ge 0$ since γ_Λ and $\gamma_\Lambda^{(n,\lambda)}$ are positivity preserving, i.e., $\gamma_\Lambda f \ge 0$ and $\gamma_\Lambda^{(n,\lambda)} \ge 0$ whenever $f \ge 0$. We notice that since the interaction Φ is of finite range, if $\gamma = 0$ then,

$$\gamma_\Lambda^{(n,0)} f(t) = \gamma_\Lambda f(t), \quad t \in \Omega_{T_n}. \tag{3.24}$$

On the other hand, since F is bounded, it is easy to see that

$$e^{-2|\lambda|\,|\Lambda|\,|\widetilde{\Lambda}|\,\|F\|_\infty} \gamma_\Lambda^{(n,0)} f(t) \le \gamma_\Lambda^{(n,\lambda)} f(t) \le e^{2|\lambda|\,|\Lambda|\,|\widetilde{\Lambda}|\,\|F\|_\infty} \gamma_\Lambda^{(n,0)} f(t) \tag{3.25}$$

From (3.24)-(3.25) we see that there exists $\lambda_0 > 0$ such that $\|F^{(n,\lambda)} - F\|_\infty \le \varepsilon$ if $|\lambda| \le \lambda_0$. Thus, our assertion (3.20) is proved.

Now, suppose that the equality (2.18) holds. Recall the notion of the pressure for general b.c. in (2.13). We see that

$$\begin{aligned}\frac{d}{d\lambda}\,{}_P P_{T_n}^{\Phi+\lambda\Psi} &= <\exp[-{}_P H_{T_n}^{\Phi+\lambda\Psi}]>_0^{-1}< -F\exp[-{}_P H_{T_n}^{\Phi+\lambda\Psi}]>_0 \\ &= < -F >_{n,\lambda}\,.\end{aligned} \tag{3.26}$$

Thus, by using (3.20) we get

$$|\frac{d}{d\lambda}\,{}_P P_{T_n}^{\Phi+\lambda\Psi}| \le \varepsilon \quad \text{for } |\lambda| \le \lambda_0. \tag{3.27}$$

This implies that

$${}_P P_{T_n}^{\Phi+\lambda\Psi} \le {}_P P_{T_n}^{\Phi} + \varepsilon|\lambda| \quad \text{for } |\lambda| \le \lambda_0. \tag{3.28}$$

By letting n go to infinity and using Theorem 2.5 we then have

$$P^{\Phi+\lambda\Psi} \le P^{\Phi} + \varepsilon|\lambda| \quad \text{for } |\lambda| \le \lambda_0. \tag{3.29}$$

On the other hand, by the same method used in the proof of (3.8), and using (2.18) we see that for any $\lambda \in \mathbb{R}$

$$\begin{aligned}P^{\Phi+\lambda\Psi} &\ge s(\mu) - \liminf_{\Lambda\to\mathbb{Z}^\nu \text{ (van Hove)}} \tfrac{1}{|\Lambda|}\mu(H_\Lambda^{\Phi+\lambda\Psi}) \\ &= s(\mu) - \lim_{\Lambda\to\mathbb{Z}^\nu \text{ (van Hove)}} \tfrac{1}{|\Lambda|}\mu(H_\Lambda^{\Phi}) - \lambda\mu(F) \\ &= P^\Phi - \lambda\mu(F).\end{aligned} \tag{3.30}$$

Combining (3.29) and (3.30) we have

$$|\mu(F)| \le \varepsilon. \tag{3.31}$$

Since $\varepsilon > 0$ is arbitrary this implies $\mu(F) = 0$, which is the equation (3.17) that was to be shown. ■

4. Proofs of Main Results: Quantum Systems

In this section we prove Theorem 2.12, that is, the state ω on $\mathcal{A}$ defined in (2.33), which satisfies the (weak) KMS condition, satisfies the Gibbs variational equality. Let us begin with some lemmas that will be needed.

Lemma 4.1. *(Jensen's inequality) Let ρ be any state on $\mathcal{A}$. Then for any self-adjoint $B \in \mathcal{A}$, $e^{\rho(B)} \le \rho(e^B)$.*

The proof of the above lemma can be found, e.g., in [Is, Lemma I.3.1].

Recall the definition of entropy for states in (2.35).

Lemma 4.2. *Suppose that ρ is a state on $\mathcal{A}$ such that the restriction ρ_Λ of ρ to any $\mathcal{A}_\Lambda$, $\Lambda \subset\subset \mathbb{Z}^\nu$, is a normal state with a density matrix $\rho^{(\Lambda)} \in \mathcal{A}_\Lambda$. Then, the following properties hold:*

(a) $S_\Lambda(\rho) \geq 0$ (positivity).

(b) $\Lambda \cap \Lambda' = \emptyset \Longrightarrow S_{\Lambda\cup\Lambda'}(\rho) \leq S_\Lambda(\rho) + S_{\Lambda'}(\rho)$ (subadditivity).

Proof. (a) is obvious since $\mathrm{Tr}_\Lambda(\rho^{(\Lambda)}) = 1$. For (b), we notice that the bound

$$\mathrm{Tr}(A\log A) - \mathrm{Tr}(A\log B) \geq \mathrm{Tr}(A - B) \tag{4.1}$$

holds for any trace class non-singular positive operators A and B. By letting $A := \rho^{(\Lambda\cup\Lambda')}$ and $B := \rho^{(\Lambda)} \otimes \rho^{(\Lambda')}$ in (4.1) we get

$$\begin{aligned} S_{\Lambda\cup\Lambda'}(\rho) &= -\mathrm{Tr}_{(\Lambda\cup\Lambda')}(A\log A) \\ &\leq -\mathrm{Tr}_{(\Lambda\cup\Lambda')}(A\log B) \\ &= -\mathrm{Tr}_\Lambda(\rho^{(\Lambda)}\log\rho^{(\Lambda)}) - \mathrm{Tr}_{\Lambda'}(\rho^{(\Lambda')}\log\rho^{(\Lambda')}) \\ &= S_\Lambda(\rho) + S_{\Lambda'}(\rho). \quad \blacksquare \end{aligned}$$

Proof of Proposition 2.10. (b) is a simple consequence of the subadditivity of entropy in Lemma 4.2 (b). In order to prove (a) let $\{e_j\}$ be the normalized eigen-vectors of $\rho^{(\Lambda)}$ with $\rho^{(\Lambda)}e_j = \lambda_j e_j$. We notice that $\sum_j \lambda_j = 1$. Then,

$$\begin{aligned} e^{S_\Lambda(\rho)-\rho(H_\Lambda)} &= e^{\mathrm{Tr}_\Lambda(\rho^{(\Lambda)}(-\log\rho^{(\Lambda)}-H_\Lambda))} \\ &= \exp\big[\sum_j \lambda_j(-\log\lambda_j - <e_j, H_\Lambda e_j>)\big] \\ &\leq \sum_j \exp[<e_j, -H_\Lambda e_j>] \quad \text{(by Jensen's inequality)} \\ &\leq \sum_j <e_j, e^{-H_\Lambda}e_j> \quad \text{(by Lemma 4.1)} \\ &= \mathrm{Tr}_\Lambda(e^{-H_\Lambda}) = e^{|\Lambda|P_\Lambda}. \quad \blacksquare \end{aligned}$$

We are now going to prove Theorem 2.12. For that purpose we need to define some notations. Recall the local Gibbs states ω_Λ defined in (2.29). We simply write ω_n for ω_{Λ_n}, where $\{\Lambda_n\}$ is a net in (2.32). We notice that the state ω in (2.33) is a weak limit of $\{\omega_n\}$. Let us write

$$K^{(n)} := \frac{1}{Z_{\Lambda_n}}\exp(-H_{\Lambda_n}) \tag{4.2}$$

and $\omega^{(\Lambda)}$ the density matrix of the restriction of ω to $\mathcal{A}_\Lambda$. When $\mathcal{H}_1$ and $\mathcal{H}_2$ are two Hilbert spaces and if A is a trace class operator on $\mathcal{H}_1 \otimes \mathcal{H}_2$ we denote by $\mathrm{Tr}_{(\mathcal{H}_1\otimes\mathcal{H}_2|\mathcal{H}_1)}(A)$ the partial trace of A on $\mathcal{H}_2$, i.e., $\mathrm{Tr}_{(\mathcal{H}_1\otimes\mathcal{H}_2|\mathcal{H}_1)}(A)$ is a trace class operator on $\mathcal{H}_1$ such that

$$\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{(\mathcal{H}_1\otimes\mathcal{H}_2|\mathcal{H}_1)}(A)) = \mathrm{Tr}_{\mathcal{H}_1\otimes\mathcal{H}_2}(A).$$

When $\Lambda \subset \Lambda'$, we simply write $\mathrm{Tr}_{(\Lambda'|\Lambda)}(A)$ for $\mathrm{Tr}_{(\mathcal{H}_{\Lambda'}|\mathcal{H}_\Lambda)}(A)$. One notes that

$$\omega^{(\Lambda)} = \text{w-}\lim_{n\to\infty} \mathrm{Tr}_{(\Lambda'|\Lambda)} K^{(n)}, \tag{4.3}$$

where w-limit means that

$$\mathrm{Tr}_\Lambda(\omega^{(\Lambda)}A) = \lim_{n\to\infty} \mathrm{Tr}_\Lambda((\mathrm{Tr}_{(\Lambda_n|\Lambda)} K^{(n)})A), \quad A \in \mathcal{A}_\Lambda. \tag{4.4}$$

We further simplify the notation $\mathrm{Tr}_{(\Lambda_n|\Lambda)} K^{(n)}$ by $K_\Lambda^{(n)}$ and $\mathrm{Tr}_{(\Lambda_n|\Lambda_n\setminus\Lambda)} K^{(n)}$ by $K_{\Lambda_n\setminus\Lambda}^{(n)}$.

Proof of Theorem 2.12. By Corollary 2.11, it is enough to show

$$s(\omega) \geq \limsup_{a\to\infty} a^{-\nu}\omega(H_{C_a}) + P^\Phi. \tag{4.5}$$

By the inequality (4.1), the subadditivity of entropy in Lemma 4.2 (b), and (2.36)-(2.37), we see that

$$\begin{aligned}
S_\Lambda(\omega) &= -\mathrm{Tr}_\Lambda(\omega^{(\Lambda)} \log \omega^{(\Lambda)}) \\
&= -\lim\nolimits_{n\to\infty} \mathrm{Tr}_\Lambda(K_\Lambda^{(n)} \log \omega^{(\Lambda)}) \\
&\geq -\limsup\nolimits_{n\to\infty} \mathrm{Tr}_\Lambda(K_\Lambda^{(n)} \log K_\Lambda^{(n)}) \\
&= \limsup\nolimits_{n\to\infty} S_\Lambda(\omega_n) \\
&\geq \limsup\nolimits_{n\to\infty}[S_{\Lambda_n}(\omega_n) - S_{\Lambda_n\setminus\Lambda}(\omega_n)] \\
&\geq \limsup\nolimits_{n\to\infty}[\omega_n(H_{\Lambda_n}) + |\Lambda_n|P_{\Lambda_n} - \omega_n(H_{\Lambda_n\setminus\Lambda}) - |\Lambda_n \setminus \Lambda| P_{\Lambda_n\setminus\Lambda}].
\end{aligned} \tag{4.6}$$

Recall the definition of the measure $d\lambda$ on the path spaces appeared in (2.27) and define for $0 \leq \alpha \leq 1$,

$$Z_{\Lambda_n}(\alpha) := \int d\lambda(s_{\Lambda_n}) \exp[-V(s_\Lambda) - V(s_{\Lambda_n\setminus\Lambda}) - \alpha W(s_\Lambda, s_{\Lambda_n\setminus\Lambda})]. \tag{4.7}$$

Notice that

$$\begin{aligned}
&\log Z_{\Lambda_n}(1) = \log Z_{\Lambda_n} = |\Lambda_n| P_{\Lambda_n} \\
&\log Z_{\Lambda_n}(0) = \log Z_\Lambda + \log Z_{\Lambda_n\setminus\Lambda} = |\Lambda| P_\Lambda + |\Lambda_n \setminus \Lambda| P_{\Lambda_n\setminus\Lambda}.
\end{aligned} \tag{4.8}$$

Using (4.8) in the last expression of (4.6) we get

$$S_\Lambda(\omega) \geq \limsup_{n\to\infty}[\omega_n(H_\Lambda) + |\Lambda|P_\Lambda + \omega_n(W(x_\Lambda, x_{\Lambda_n\setminus\Lambda})) + \log Z_{\Lambda_n}(1) - \log Z_{\Lambda_n}(0)]. \tag{4.9}$$

In Appendix, we will show that there exists $c > 0$ such that the bounds

$$\begin{aligned}
\limsup\nolimits_{n\to\infty} |\omega_n(W(x_\Lambda, x_{\Lambda_n\setminus\Lambda}))| &\leq c \sum_{i\in\Lambda}\sum_{j\in\Lambda^c} \Psi(|i-j|), \\
\limsup\nolimits_{n\to\infty} |\log Z_{\Lambda_n}(1) - \log Z_{\Lambda_n}(0)| &\leq c \sum_{i\in\Lambda}\sum_{j\in\Lambda^c} \Psi(|i-j|)
\end{aligned} \tag{4.10}$$

hold. Using (4.10) in (4.9) we get

$$S_\Lambda(\omega) \geq \omega(H_\Lambda) + |\Lambda|P_\Lambda - 2c\sum_{i\in\Lambda}\sum_{j\in\Lambda^c}\Psi(|i-j|). \tag{4.11}$$

We take Λ to be the cubes C_a of sides a and divide both sides of (4.11) by $a^{-\nu}$, the volume of C_a, and use (2.38), Theorem 2.8, and the method used to show (3.11) to get the inequality (4.5). The proof is now completed. ■

Appendix.

We show the inequlities in (4.10). We first prove the second inequality of (4.10). By the mean value theorem there exists $\alpha_1 \in (0,1)$ such that

$$\begin{aligned}
&\log Z_{\Lambda_n}(1) - \log Z_{\Lambda_n}(0)\\
&= \frac{d}{d\alpha}\log Z_{\Lambda_n}(\alpha)\Big|_{\alpha=\alpha_1}\\
&= \frac{1}{Z_{\Lambda_n}(\alpha_1)}\int d\lambda(s_{\Lambda_n})\exp[-V(s_\Lambda) - V(s_{\Lambda_n\setminus\Lambda}) - \alpha_1 W(s_\Lambda, s_{\Lambda_n\setminus\Lambda})](-W(s_\Lambda, s_{\Lambda_n\setminus\Lambda}))\\
&=:< -W(s_\Lambda, s_{\Lambda_n\setminus\Lambda}) >_{\alpha_1},
\end{aligned} \tag{A.1}$$

where the expectation $< \cdot >_\alpha$, $0 \leq \alpha \leq 1$, is defined by

$$< A >_\alpha := \frac{1}{Z_{\Lambda_n}(\alpha)}\int d\lambda(s_{\Lambda_n})\exp[-V(s_\Lambda) - V(s_{\Lambda_n\setminus\Lambda}) - \alpha W(s_\Lambda, s_{\Lambda_n\setminus\Lambda})]A(s_{\Lambda_n}). \tag{A.2}$$

We then have

$$\frac{d^2}{d\alpha^2}\log Z_{\Lambda_n}(\alpha) =< W(s_\Lambda, s_{\Lambda_n\setminus\Lambda})^2 >_\alpha - < W(s_\Lambda, s_{\Lambda_n\setminus\Lambda}) >_\alpha^2 \geq 0.$$

That is, the function $\alpha \mapsto \frac{d}{d\alpha}\log Z_{\Lambda_n}(\alpha)$ is a monotone function and hence we have

$$|\log Z_{\Lambda_n}(1) - \log Z_{\Lambda_n}(0)| \leq \max\Big\{\Big|\frac{d}{d\alpha}\log Z_{\Lambda_n}(\alpha)\Big|_{\alpha=0}\Big|,\ \Big|\frac{d}{d\alpha}\log Z_{\Lambda_n}(\alpha)\Big|_{\alpha=1}\Big|\Big\}. \tag{A.3}$$

We calculate $\frac{d}{d\alpha}\log Z_{\Lambda_n}(\alpha)\big|_{\alpha=1}$. The other one can be done similary. First, notice that by a superstable estimate established in [PY, Proposition 2.5], there exist $A^* > 0$ and $\delta > 0$ such that for any $\Delta \subset \Lambda_n$,

$$\frac{1}{Z_{\Lambda_n}}\int d\lambda(s_{\Lambda_n\setminus\Delta})e^{-V(s_{\Lambda_n})} \leq \exp\big[\sum_{i\in\Delta}(-A^* s_i^2 + \delta)\big]. \tag{A.4}$$

Then, by the regularity of the interaction given in Assumption 2.1 (d) we see that

$$\begin{aligned}
&\Big|\frac{d}{d\alpha}\log Z_{\Lambda_n}(\alpha)\Big|_{\alpha=1}\Big| \\
&=\Big|\frac{1}{Z_{\Lambda_n}}\int d\lambda(s_{\Lambda_n})e^{-V(s_{\Lambda_n})}W(s_\Lambda, s_{\Lambda_n\setminus\Lambda})\Big| \\
&\le \sum_{i\in\Lambda}\sum_{j\in\Lambda_n\setminus\Lambda}\frac{1}{2}\Psi(|i-j|)\frac{1}{Z_{\Lambda_n}}\int d\lambda(s_{\Lambda_n})e^{-V(s_{\Lambda_n})}(s_i^2+s_j^2) \\
&\le \sum_{i\in\Lambda}\sum_{j\in\Lambda_n\setminus\Lambda}\frac{1}{2}\Psi(|i-j|)\int d\lambda(s_i)d\lambda(s_j)e^{-A^*(s_i^2+s_j^2)+2\delta}(s_i^2+s_j^2) \\
&\le c\sum_{i\in\Lambda}\sum_{j\in\Lambda_n\setminus\Lambda}\Psi(|i-j|).
\end{aligned}$$

In order to prove the first inequality of (4.10) we notice, by using the regularity of the interaction and (A.4), that

$$\begin{aligned}
&|\omega_n(W(x_\Lambda, x_{\Lambda_n\setminus\Lambda}))| \\
&=\Big|\frac{1}{Z_{\Lambda_n}}\int d\lambda(s_{\Lambda_n})e^{-V(s_{\Lambda_n})}W(x_\Lambda, x_{\Lambda_n\setminus\Lambda})\Big| \\
&\le \sum_{i\in\Lambda}\sum_{j\in\Lambda_n\setminus\Lambda}\frac{1}{2}\Psi(|i-j|)\int d\lambda(s_i)d\lambda(s_j)e^{-A^*(s_i^2+s_j^2)+2\delta}(s_i(0)^2+s_j(0)^2).
\end{aligned} \tag{A.5}$$

Notice that

$$\int d\lambda(s_i)e^{-A^*s_i^2}s_i(0)^2=\int dx_i\, x_i^2\int P_{x_i,x_i}(ds_i)e^{-A^*s_i^2}. \tag{A.6}$$

By using the same argument used in the proof of the bounds in (A.13)-(A.15) of [PY], we get that the r.h.s. of (A.6) is bounded by

$$\int dx_i\, x_i^2 e^{-A'x_i^2+\delta'}\le c'<\infty, \tag{A.7}$$

for some constants A', δ', and c'. Inserting (A.7) into (A.5) we finish the proof of (4.10).

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