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A NOTE ON THE NON-COMMUTATIVE LAPLACE–VARADHAN INTEGRAL LEMMA

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We continue the study of the free energy of quantum lattice spin systems where to the local Hamiltonian H an arbitrary mean field term is added, a polynomial function of the arithmetic mean of some local observables X and Y that do not necessarily commute. By slightly extending a recent paper by Hiai, Mosonyi, Ohno and Petz [10], we prove in general that the free energy is given by a variational principle over the range of the operators X and Y. As in [10], the result is a non-commutative extension of the Laplace–Varadhan asymptotic formula.

Keywords: Quantum large deviations; quantum lattice systems; Laplace–Varadhan lemma.

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1. Introduction

1.1. *Large deviations*

One of the highlights in the combination of analysis and probability theory is the asymptotic evaluation of certain integrals. We have here in mind integrals of the form, for some real-valued function G,

$$\int \mathrm{d}\mu_n(x) \exp\{v_n G(x)\}, \quad v_n \nearrow +\infty \quad \text{as } n \nearrow +\infty \tag{1.1}$$

for which the measures μ_n satisfy a law of large numbers. Such integrals can be evaluated depending on the asymptotics of the μ_n. The latter is the subject of the theory of large deviations, characterizing the rate of convergence in the law of large numbers. In a typical scenario, the μ_n are the probabilities of some macroscopic variable, such as the average magnetization or the particle density in ever growing volumes v_n and as distributed in a given equilibrium Gibbs ensemble. Then, depending on the case, thermodynamic potentials $\mathcal{J}$ make the rate function $\mathrm{d}\mu_n(x) \sim \mathrm{d}x \exp\{-v_n\mathcal{J}(x)\}$ in the sense of large deviations for Gibbs measures, see [8, 9, 16, 22, 23]. That theory of large deviations is however broader than the applications in equilibrium statistical mechanics. Essentially, when the rate function for μ_n is given by $\mathcal{J}$, then the integral (1.1) is computed as

$$\frac{1}{v_n} \log \int \mathrm{d}\mu_n(x) \exp\{v_n G(x)\} \xrightarrow[n\nearrow+\infty]{} \sup_x \{G(x) - \mathcal{J}(x)\}. \tag{1.2}$$

This is a typical application of Laplace's asymptotic formula for the evaluation of real-valued integrals. The systematic combination with the theory of large deviations gives the so called Laplace–Varadhan integral lemma.

We first recall the large deviation principle (LDP). Let (M, d) be some complete separable metric space.

Definition 1.1. The sequence of measures μ_n on M satisfies a LDP with rate function $\mathcal{J} : M \to \mathbb{R}^+ \cup \{+\infty\}$ and speed $v_n \in \mathbb{R}^+$ if

(1) $\mathcal{J}$ is convex and has closed level sets, i.e.

$$\{\mathcal{J}^{-1}(x), x \leq c\} \tag{1.3}$$

is closed in (M, d) for all $c \in \mathbb{R}^+$;

(2) for all Borel sets $U \subset M$ with interior $\operatorname{int} U$ and closure $\operatorname{cl} U$, one has

$$\liminf_{n\nearrow+\infty} \frac{1}{v_n} \log \mu_n(U) \geq - \inf_{u\in \operatorname{int} U} \mathcal{J}(u),$$

$$\limsup_{n\nearrow+\infty} \frac{1}{v_n} \log \mu_n(U) \leq - \inf_{u\in \operatorname{cl} U} \mathcal{J}(u).$$

We say that the rate function $\mathcal{J}$ is *good* whenever the level sets (1.3) are compact.

For the transfer of LDP, one considers a pair (μ_n, ν_n), $n \nearrow \infty$ of sequences of absolutely continuous measures on (M, d) such that

$$\frac{\mathrm{d}\nu_n}{\mathrm{d}\mu_n}(x) = \exp\{v_n\, G(x)\}, \quad \mu_n\text{-almost everywhere,}$$

for some measurable mapping $G : M \to \mathbb{R}$. We now state an instance of the Laplace–Varadhan lemma.

Lemma 1.1 (Laplace–Varadhan Integral Lemma). *Assume that G is bounded and continuous and that the sequence (μ_n) satisfies a large deviation principle with good rate function $\mathcal{J}$ and speed v_n. Then (ν_n) satisfies a large deviation principle with good rate function $G - \mathcal{J}$ and speed v_n.*

For more general versions and proofs we refer to the literature, see e.g. [5–7, 22, 23]; it remains an important subject of analytic probability theory to extend the validity of the variational formulation (1.2) and to deal with its applications.

1.2. *Mean-field interactions*

From the point of view of equilibrium statistical mechanics, one can also think of the formula (1.1) as giving (the exponential of) the pressure or free energy when adding a mean field type term to a Hamiltonian which is a sum of local interactions.

The choice of the function G is then typically monomial with a power decided by the number of particles or spins that are in direct interaction. For example, the free energy of an Ising-like model with such an extra mean field interaction would be given by the limit

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \sum_{\eta \in \{+,-\}^\Lambda} \exp\left(-\beta H_\Lambda(\eta) + \lambda_p |\Lambda| \left(\frac{1}{|\Lambda|} \sum_{i \in \Lambda} \eta_i \right)^p \right) \tag{1.4}$$

for $p = 1, 2, \ldots$, where $H_\Lambda(\eta)$ is the (local) energy of the spin configuration η and the limit takes a sequence of regularly expanding boxes Λ to cover some given lattice. The case $p = 1$ corresponds to the addition of a magnetic field λ_1; $p = 2$ is most standard and adds effectively a very small but long range two-spin interaction. Higher p-values are also not uncommon in the study of Ising interactions on hypergraphs, and even very large p has been found relevant, e.g., in models of spin glasses and in information theory [4].

The form (1.1) is easily recognized in (1.4), with

$$\mu_n(x) \sim \sum_{\eta \in \{+,-\}^\Lambda, \sum_{i\in\Lambda} \eta_i = x|\Lambda|} \exp\{-\beta H_\Lambda(\eta)\}, \quad v_n = |\Lambda|,$$

and the function $G(x) = \lambda_p x^p$. The Laplace–Varadhan lemma applies to (1.4) since we know that the sequence of Gibbs states with density $\sim \exp\{-\beta H_\Lambda(\,\cdot\,)\}$ satisfies a LDP with a good rate function $\mathcal{J}_{\text{cl}}$ and speed $|\Lambda|$. The result reads that (1.4) is given by the variational formula

$$\sup_{u \in [-1,1]} \{\lambda_p u^p - \mathcal{J}_{\text{cl}}(u)\}. \tag{1.5}$$

In non-commutative versions the local Hamiltonian H and the additional mean field term are allowed not to commute with each other. That is natural within the statistical mechanics of quantum spin systems and this is also the context of the present paper.

1.3. *Non-commutative extensions*

Although it has proven very useful to think of integrals (1.1) within the framework of probability and large deviation theory, it is fundamentally a problem of analysis. However, without such a probabilistic context, the question of a non-commutative extension of the Laplace–Varadhan Lemma 1.1 becomes ambiguous and it in fact allows for different formulations, each possibly having a physical interpretation on its own.

One approach is to ask for the asymptotic evaluation of the expectations

$$\lim_{\Lambda\nearrow\mathbb{Z}^d} \frac{1}{|\Lambda|} \log \omega_\Lambda(e^{|\Lambda|\, G(\bar{X}_\Lambda)}) \tag{1.6}$$

under a family of quantum states ω_Λ where $\bar{X}_\Lambda$ would now be the arithmetic mean of some quantum observable in volume Λ. To be specific, one can take ω_Λ a quantum Gibbs state for a Hamiltonian H_Λ at inverse temperature β, with density matrix $\sigma_\Lambda \sim \exp\{-\beta H_\Lambda\}$, and $\bar{X}_\Lambda = (\sum_{i\in\Lambda} X_i)/|\Lambda|$ the mean magnetization in some fixed direction. Arguably, this formulation is closely related to the asymptotic statistics of outcomes in von Neumann measurements of $\bar{X}_\Lambda$. Indeed, let ν_Λ be the measure on $[-\|X\|, \|X\|]$ defined by

$$\nu_\Lambda(f) := \omega_\Lambda(f(\bar{X}_\Lambda)) \quad \text{for } f \in \mathcal{C}([-\|X\|, \|X\|]). \tag{1.7}$$

Then, (1.6) can be evaluated with the help of Lemma 1.1 (the *commutative* Laplace–Varadhan integral lemma) if the family ν_Λ satisfies a LDP with speed $|\Lambda|$. In recent years, this LDP has been established for $\sigma_\Lambda \sim \exp\{-\beta H_\Lambda\}$ in the regime of small β (high temperature) or $d = 1$, see [11, 13–15].

A more general class of possible extensions is obtained by considering the limits of

$$\frac{1}{|\Lambda|} \log \mathrm{Tr}_\Lambda(\sigma_\Lambda^{\frac{1}{K}}\, e^{\frac{|\Lambda|}{K} G(\bar{X}_\Lambda)})^K, \quad \Lambda \nearrow \mathbb{Z}^d \tag{1.8}$$

for different $K > 0$, where σ_Λ is the density matrix of a quantum state in box Λ. For the canonical form $\sigma_\Lambda = \exp(-\beta H_\Lambda)/Z_\Lambda^\beta$ with local Hamiltonian H_Λ at inverse temperature β, (1.8) becomes

$$\frac{1}{|\Lambda|} \log \frac{1}{Z_\Lambda^\beta} \mathrm{Tr}_\Lambda(e^{-\frac{\beta}{K} H_\Lambda}\, e^{\frac{|\Lambda|}{K}\, G(\bar{X}_\Lambda)})^K, \quad \Lambda \nearrow \mathbb{Z}^d. \tag{1.9}$$

There is no *a priori* reason to exclude any particular value of K from consideration. Two standard options are: $K = 1$, which corresponds to the expression (1.6) above, and $K \nearrow +\infty$, which, by the Trotter product formula, boils down to

$$\frac{1}{|\Lambda|} \log \frac{1}{Z_\Lambda^\beta} \mathrm{Tr}_\Lambda(e^{-\beta H_\Lambda + |\Lambda| G(\bar{X}_\Lambda)}), \quad \Lambda \nearrow \mathbb{Z}^d \tag{1.10}$$

which is the free energy of a corresponding quantum spin model, cf. (1.4). In the present paper, we study the case $K \nearrow +\infty$ (without touching the question of interchangeability of both limits).

One of our results, Theorem 3.1 with $Y = \bar{Y}_\Lambda = 0$, is of the form

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{Tr}_\Lambda (e^{-\beta H_\Lambda + |\Lambda|\, G(\bar{X}_\Lambda)}) = \sup_{-\|X\| \le u \le \|X\|} \{G(u) - \mathcal{J}(u)\}. \tag{1.11}$$

Note that we omitted the normalization factor $1/Z_\Lambda^\beta$ since it merely adds a constant (independent of G) to (1.10). In the usual context of the theory of large deviations, formula (1.11) arises as a change of rate function. However, while our result (1.11) very much looks like Varadhan's formula in Lemma 1.1, there is a big difference in interpretation: The function $\mathcal{J}$ is not as such the rate function of large deviations for $\bar{X}_\Lambda$. Instead, it is given as the Legendre transform

$$\mathcal{J}(u) = \sup_{t \in \mathbb{R}} \{tu - q(t)\}, \quad u \in \mathbb{R} \tag{1.12}$$

of a function $q(\,\cdot\,)$ which is the pressure corresponding to a linearized interaction, i.e.

$$q(t) = \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{Tr}_\Lambda (e^{-\beta H_\Lambda + t|\Lambda| \bar{X}_\Lambda}). \tag{1.13}$$

1.4. *Several non-commuting observables: Towards joint large deviations?*

In the previous Sec. 1.3, we made the tacit assumption that there is a single observable $\bar{X}_\Lambda$ corresponding to some Hermitian operator on Hilbert space. However, in formula (1.4), the observable $\frac{1}{|\Lambda|} \sum_{i \in \Lambda} \eta_i$ could equally well represent a vector-valued magnetization which, upon quantization, would correspond to several non-commuting observables $\bar{X}_\Lambda, \bar{Y}_\Lambda$, say, the magnetization along the x-axis and y-axis, respectively. In the commutative theory, this case does not require special attention; the framework of large deviations applies equally regardless of whether the observable takes values in $\mathbb{R}$ or $\mathbb{R}^2$. Obviously, this is not true in the non-commutative setting and in fact, we do not even know a natural analogue of the generating function (1.6), since we do not dispose of a simultaneous Von Neumann measurement of $\bar{X}_\Lambda$ and $\bar{Y}_\Lambda$. One can take the point of view that this is inevitable in quantum mechanics, and insisting is pointless. Yet, as $\Lambda \nearrow \mathbb{Z}^d$, the commutator

$$[\bar{X}_\Lambda, \bar{Y}_\Lambda] = O\left(\frac{1}{|\Lambda|}\right) \tag{1.14}$$

vanishes and hence the joint measurability of $\bar{X}_\Lambda, \bar{Y}_\Lambda$ is restored on the macroscopic scale. We refer the reader to [19] where this issue is discussed and studied in more depth.

The advantage of the approach via the Laplace–Varadhan Lemma is that one can set aside these conceptual questions and study joint large deviations of $\bar{X}_\Lambda$ and $\bar{Y}_\Lambda$ by choosing G to be a joint function of $\bar{X}_\Lambda$ and $\bar{Y}_\Lambda$, for example a symmetrized monomial

$$G(\bar{X}_\Lambda, \bar{Y}_\Lambda) = (\bar{X}_\Lambda)^k (\bar{Y}_\Lambda)^l + (\bar{Y}_\Lambda)^l (\bar{X}_\Lambda)^k, \quad \text{for some } k, l \in \mathbb{N}, \tag{1.15}$$

and check whether the formula (1.11) remains valid with some obvious adjustments. This turns out to be the case and it is our main result: Theorem 3.1.

1.5. *Comparison with previous results*

The asymptotics of the expression (1.10) was first studied and the result (1.11) was first obtained by Petz *et al.* [17], in the case where the Hamiltonian H_Λ is made solely from a one-body interaction. The corresponding equilibrium state is then a product state. In [10], Hiai *et al.* generalized this result to the case of locally interacting spins but the lattice dimension was restricted to $d = 1$. However, the authors of [10] argue that the restriction to $d = 1$ can be lifted in the high-temperature regime. The main reason is that their work relies heavily on an asymptotic decoupling condition which is proven in that regime, [1]. One should observe here that this asymptotic decoupling condition in fact implies a large deviation principle for $\bar{X}_\Lambda$, as follows from the work of Pfister [18]. Hence, in the language of Sec. 1.3, [10] evaluates (1.10) (the case $K = \infty$) in those regimes where (1.6) (the case $K = 1$) can be evaluated as well.

The present paper elaborates on the result of [10] in two ways. First, we remark that, in our setup, the decoupling condition is actually not necessary for (1.11) to hold, and therefore one can do away with the restriction to $d = 1$ or high temperature. Hence, again referring to Sec. 1.3, the case $K = \infty$ can be controlled even when we know little about the case $K = 1$. To drop the decoupling condition, it is absolutely essential that we start from finite-volume Gibbs states, and not from finite-volume restrictions of infinite-volume Gibbs states, as it is done in [10].

Second, we show that by the same formalism, one can treat the case of several noncommuting observables, as explained in Sec. 1.4. The most serious step in this generalization is actually an extension of the result of [17] to noncommuting observables. This extension is stated in Lemma 6.1 and proven in Sec. 7.

Note. While we were finishing this paper, we learnt of a similar project by J.-B. Bru and W. de Siqueira Pedra. Their result [3] is nothing less than a full-fledged theory of equilibrium states with mean-field terms in the Hamiltonian, describing not only the mean-field free energy (as we do here), but also the states themselves. Also, their results hold for fermions, while ours are restricted to spin systems, and they provide interesting examples. Yet, the focus of our paper differs from theirs and our main result is not contained in their paper.

1.6. *Outline*

In Sec. 2, we sketch the setup. We introduce spin systems on the lattice, noncommutative polynomials and ergodic states. Section 3 describes the result of the paper. The remaining Secs. 4–7 contain the proofs.

2. Setup

2.1. *Hamiltonian and observables*

We consider a quantum spin system on the regular lattice $\mathbb{Z}^d$, $d = 1, 2, \ldots$. We briefly introduce the essential setup below, and we refer to [12, 20] for more expanded, standard introductions.

The single site Hilbert space $\mathcal{H}$ is finite-dimensional (isomorphic to $\mathbb{C}^n$) and for any finite volume $\Lambda \subset \mathbb{Z}^d$, we set $\mathcal{H}_\Lambda = \otimes_\Lambda \mathcal{H}$. The C^*-algebra of bounded operators on $\mathcal{H}_\Lambda$ is denoted by $\mathcal{B}_\Lambda \equiv \mathcal{B}(\mathcal{H}_\Lambda)$. The standard embedding $\mathcal{B}_\Lambda \subset \mathcal{B}_{\Lambda'}$ for $\Lambda \subset \Lambda'$ is assumed throughout. The quasi-local algebra $\mathfrak{U}$ is defined as the norm closure of the finite-volume algebras

$$\mathfrak{U} := \overline{\bigcup_{\Lambda\,\text{finite}} \mathcal{B}_\Lambda}. \tag{2.1}$$

Denote by τ_i, $i \in \mathbb{Z}^d$, the translation which shifts all observables over a lattice vector i, i.e. τ_i is a homomorphism from $\mathcal{B}_\Lambda$ onto $\mathcal{B}_{i+\Lambda}$.

We introduce an interaction potential Φ, that is a collection (Φ_A) of Hermitian elements of $\mathcal{B}_A$, labeled by finite subsets $A \subset \mathbb{Z}^d$. We assume translation invariance (i) and a finite range (ii):

(i) $\tau_i(\Phi_A) = \Phi_{i+A}$ for all finite $A \subset \mathbb{Z}^d$;
(ii) there is a $d_{\max} < \infty$ such that, if $\operatorname{diam}(A) > d_{\max}$, then $\Phi_A = 0$.

In estimates, we will frequently use the number

$$r(\Phi) := \sum_{A \ni 0} \|\Phi_A\| < \infty. \tag{2.2}$$

The local Hamiltonian in a finite volume Λ is

$$H_\Lambda \equiv H_\Lambda^\Phi = \sum_{A \subset \Lambda} \Phi_A \tag{2.3}$$

which corresponds to free or open boundary conditions. Boundary conditions will however turn out to be irrelevant for our results. We will drop the superscript Φ since we will keep the interaction potential fixed.

Let $X, Y, \ldots$ denote local observables on the lattice, located at the origin, i.e. $\operatorname{Supp} X$ (which is defined as the smallest set A such that $X \in \mathcal{B}_A$) is a finite set which includes $0 \in \mathbb{Z}^d$.

We write

$$X_\Lambda := \sum_{j \in \mathbb{Z}^d, \operatorname{Supp} \tau_j X \subset \Lambda} \tau_j X \tag{2.4}$$

and

$$\bar{X}_\Lambda := \frac{1}{|\Lambda|} X_\Lambda \tag{2.5}$$

for the corresponding intensive observable (the "empirical average" of X).

All of these operators are naturally embedded into the quasi-local algebra $\mathfrak{U}$. At some point, we will also require the intensive infinite volume observable

$$\bar{X} \sim \bar{X}_{\Lambda\nearrow\infty}.$$

Some care is required in dealing with $\bar{X}$ since it does not belong to the quasi-local algebra $\mathfrak{U}$. We will further comment on this in Sec. 2.3.

2.2. *Non-commutative polynomials*

We will perturb the Hamiltonian H_Λ^Φ by a mean field term of the form $|\Lambda|G(\bar{X}_\Lambda, \bar{Y}_\Lambda)$ where G is a "non-commutative polynomial" of the operators $\bar{X}_\Lambda, \bar{Y}_\Lambda$, e.g., as in (1.15).

In this section, we introduce these non-commutative polynomials G as quantizations of polynomial functions g. First, we define

$$\mathrm{Ran}(X,Y) := [-\|X\|, \|X\|] \times [-\|Y\|, \|Y\|]. \tag{2.6}$$

This definition is motivated by the fact that ("sp" stands for spectrum)

$$\mathrm{sp}\,\bar{X}_\Lambda \times \mathrm{sp}\,\bar{Y}_\Lambda \subset \mathrm{Ran}(X,Y), \quad \text{for all } \Lambda. \tag{2.7}$$

Let g be a real polynomial function on the rectangular set $\mathrm{Ran}(X,Y)$. Using the symbol $\mathcal{I}$ for the collection of all finite sequences from the binary set $\{1,2\}$, any map $\tilde{G} : \mathcal{I} \to \mathbb{C}$ is called a quantization of g whenever

$$\sum_{n=0}^{N} \sum_{\alpha=(\alpha(1),\ldots,\alpha(n))\in\mathcal{I}} \tilde{G}(\alpha)\, x_{\alpha(1)} \cdots x_{\alpha(n)} = g(x_1, x_2) \tag{2.8}$$

for all $(x_1, x_2) \in \mathrm{Ran}(X,Y)$ and for some $N \in \mathbb{N}$. A quantization $\tilde{G}$ is called symmetric whenever

$$\overline{\tilde{G}(\alpha(1),\ldots,\alpha(n))} = \tilde{G}(\alpha(n),\ldots,\alpha(1)). \tag{2.9}$$

Any such symmetric quantization $\tilde{G}$ defines a self-adjoint operator

$$G(X,Y) = \sum_{n=0}^{N} \sum_{\alpha=(\alpha(1),\ldots,\alpha(n))\in\mathcal{I}} \tilde{G}(\alpha)\, X_{\alpha(1)} \cdots X_{\alpha(n)} \tag{2.10}$$

taking $X_1 \equiv X$ and $X_2 \equiv Y$.

In the thermodynamic limit, one expects different quantizations of g to be equivalent:

Lemma 2.1. *Let $\tilde{G}$ and $\tilde{G}'$ be any two quantizations of $g : \mathrm{Ran}(X,Y) \to \mathbb{R}$. Then*

$$\|G(\bar{X}_\Lambda, \bar{Y}_\Lambda) - G'(\bar{X}_\Lambda, \bar{Y}_\Lambda)\| \le \frac{C_g(X,Y)}{|\Lambda|} \tag{2.11}$$

for some $C_g(X,Y) < \infty$, and for all finite volumes Λ.

Proof. This is a simple consequence of the fact that the commutator of macroscopic observables vanishes in the thermodynamic limit, more precisely,

$$\|[\bar{X}_\Lambda, \bar{Y}_\Lambda]\| \leq \frac{1}{|\Lambda|}\|X\||\operatorname{Supp} X| \times \|Y\||\operatorname{Supp} Y|. \tag{2.12}$$

□

Indeed, our results, Theorems 3.1 and 3.2, do not depend on the choice of quantization. This can also be checked a priori using the above lemma and the log-trace inequality in (3.11).

2.3. *Infinite-volume states*

A state ω_Λ is a positive linear functional on $\mathcal{B}_\Lambda$, normalized by $\|\omega_\Lambda\| = \omega_\Lambda(1) = 1$. An example is the tracial state, $\omega_\Lambda(\,\cdot\,) \sim \operatorname{Tr}_\Lambda(\,\cdot\,)$. In general we consider states ω_Λ as characterized by their density matrix σ_Λ, $\omega_\Lambda(\,\cdot\,) = \operatorname{Tr}_\Lambda(\sigma_\Lambda\,\cdot)$.

An infinite volume state ω is a positive normalized function on the C^*-algebra $\mathfrak{U}$ (the quasi-local algebra). It is translation invariant when $\omega(A) = \omega(\tau_j A)$ for all $j \in \mathbb{Z}^d$ and $A \in \mathfrak{U}$. A translation-invariant state ω is *ergodic* whenever it is an extremal point in the convex set of translation invariant states. A state is called *symmetric* whenever it is invariant under a permutation of the lattice sites, that is, for any sequence of one-site observables $A_1, \ldots, A_n \in \mathcal{B}_{\{0\}} \subset \mathfrak{U}$ and $i_1, \ldots, i_n \in \mathbb{Z}^d$

$$\omega(\tau_{i_1}(A_1)\tau_{i_2}(A_2)\cdots\tau_{i_n}(A_n)) = \omega(\tau_{i_{\pi(1)}}(A_1)\tau_{i_{\pi(2)}}(A_2)\cdots\tau_{i_{\pi(n)}}(A_n)) \tag{2.13}$$

for any permutation π of the set $\{1, \ldots, n\}$. The set of ergodic/symmetric states on $\mathfrak{U}$ is denoted by $\mathcal{S}_{\mathrm{erg}}, \mathcal{S}_{\mathrm{sym}}$, respectively.

At some point we will need the theorem by Størmer [21] that states that any $\omega \in \mathcal{S}_{\mathrm{sym}}$ can be decomposed as

$$\omega = \int_{\mathrm{prod.}} \mathrm{d}\nu_\omega(\phi)\phi \tag{2.14}$$

for some regular probability measure ν_ω whose support consists of product states. Of course, the set of product states can be identified with the (finite-dimensional) set of states on the one-site algebra $\mathcal{B}_{\{0\}} = \mathcal{B}(\mathcal{H})$.

For a finite-volume state ω_Λ on $\mathcal{B}_\Lambda$, we consider the entropy functional

$$S(\omega_\Lambda) \equiv S_\Lambda(\omega_\Lambda) = -\operatorname{Tr}\sigma_\Lambda \log \sigma_\Lambda. \tag{2.15}$$

The mean entropy of a translation-invariant infinite-volume state ω is defined as

$$s(\omega) := \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} S(\omega_\Lambda), \quad \text{with } \omega_\Lambda := \omega\big|_{\mathcal{B}_\Lambda} \text{ (restriction to } \Lambda). \tag{2.16}$$

In this formula and in the rest of the paper, the limit $\lim_{\Lambda \nearrow \mathbb{Z}^d}$ is meant in the sense of *Van Hove*, see, e.g., [12, 20]. Standard properties of the functional s are its affinity and upper semicontinuity (with respect to the weak$*$-topology on states).

In Sec. 2.1, we mentioned the observables at infinity' $\bar{X}$ and $\bar{Y}$, postponing their definition to the present section. Expressions like $\omega(\bar{X}^l\bar{Y}^k)$ (for some positive numbers l, k) can be defined as

$$\omega(\bar{X}^l\bar{Y}^k) := \lim_{\Lambda,\Lambda'\nearrow\mathbb{Z}^d} \omega(\bar{X}_\Lambda^l \bar{Y}_{\Lambda'}^k), \tag{2.17}$$

provided that the limit exists. We use the following standard result that can be viewed as a non-commutative law of large numbers

Lemma 2.2. *For $\omega \in \mathcal{S}_{\mathrm{erg}}$, the limit (2.17) exists and*

$$\omega(\bar{X}^l\bar{Y}^k) = [\omega(X)]^l[\omega(Y)]^k. \tag{2.18}$$

Note that $\omega(X) = \omega(\bar{X})$ and $\omega(Y) = \omega(\bar{Y})$ by translation invariance. An immediate corollary is that for a non-commutative polynomial G which is a quantization of g (see Sec. 2.2), and $\omega \in \mathcal{S}_{\mathrm{erg}}$:

$$\omega(G(\bar{X},\bar{Y})) = g(\omega(X),\omega(Y)). \tag{2.19}$$

For the convenience of the reader, we sketch the proof of Lemma 2.2 in the Appendix.

Finally, we note that Lemma 2.2 does not require the state ω to be trivial at infinity. Triviality at infinity is a stronger notion which is not used in the present paper. In particular, the state $\bar{\mu}$ constructed in Sec. 4 is ergodic, but not trivial at infinity, since it fails to be ergodic with respect to a subgroup of lattice translations.

3. Result

Choose X, Y to be local operators and let H_Λ^Φ be the Hamiltonian corresponding to a finite-range, translation invariant interaction Φ, as in Sec. 2.1. Let $\tilde{G}$ be a symmetric quantization of a polynomial g on the rectangle $\mathrm{Ran}(X,Y)$ and $G(\,\cdot\,,\cdot\,)$ the corresponding self-adjoint operator, as defined in Sec. 2.2. We define the "G-mean field partition function"

$$Z_\Lambda^G(\Phi) := \mathrm{Tr}_\Lambda(e^{-H_\Lambda+|\Lambda|\,G(\bar{X}_\Lambda,\bar{Y}_\Lambda)}) \tag{3.1}$$

with $\bar{X}_\Lambda, \bar{Y}_\Lambda$ empirical averages of X, Y. The following theorem is our main result:

Theorem 3.1. *Define the pressure*

$$p(u,v) = \lim_{\Lambda\nearrow\mathbb{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{Tr}_\Lambda\, e^{-H_\Lambda^\Phi + uX_\Lambda + vY_\Lambda} \tag{3.2}$$

and its Legendre transform

$$I(x,y) = \sup_{(u,v)\in\mathbb{R}^2} (ux + vy - p(u,v)). \tag{3.3}$$

Then

$$\lim_{\Lambda\nearrow\mathbb{Z}^d} \frac{1}{|\Lambda|} \log Z_\Lambda^G(\Phi) = \sup_{(x,y)\in\mathbb{R}^2} (g(x,y) - I(x,y)) \tag{3.4}$$

where the limit $\Lambda \nearrow \mathbb{Z}^d$ is in the sense of Van Hove, as in (3.2)*. In particular, the left-hand side of* (3.4) *does not depend on the particular form of quantization taken.*

As discussed in Sec. 1, our result expresses the pressure of the mean field Hamiltonian through a variational principle. To derive this result, it is helpful to represent this pressure first as a variational problem on a larger space, namely that of ergodic states, as in Theorem 3.2. Theorem 3.1 follows then by parametrizing these states by their values on X and Y.

We also need the "local energy operator" associated to the interaction Φ as

$$E_\Phi := \sum_{A \ni 0} \frac{1}{|A|} \Phi_A. \tag{3.5}$$

Theorem 3.2 (Mean-Field Variational Principle). *Let $s(\cdot)$ be the mean entropy functional, as in Sec.* 2.3*. Then*

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log Z_\Lambda^G(\Phi) = \sup_{\omega \in \mathcal{S}_{\mathrm{erg}}} (g(\omega(X), \omega(Y)) + s(\omega) - \omega(E_\Phi)). \tag{3.6}$$

To understand how the first term on the right-hand side of (3.6) originates from (3.1), we recall the equality (2.19) for ergodic states ω.

The proof of Theorem 3.2 is postponed to Secs. 5 and 6. Here we prove that Theorem 3.1 is a rather immediate consequence of Theorem 3.2.

Proof of Theorem 3.1. We write the right-hand side of (3.6) in the form

$$\sup_{(x,y) \in \mathbb{R}^2} (g(x,y) - \tilde{I}(x,y)) \tag{3.7}$$

where

$$\tilde{I}(x,y) = \inf_{\substack{\omega \in \mathcal{S}_{\mathrm{erg}} \\ \omega(X)=x,\, \omega(Y)=y}} (-s(\omega) + \omega(E_\Phi)) \tag{3.8}$$

is a convex function on $\mathbb{R}^2$, infinite on the complement of $\mathrm{Ran}(X, Y)$. To establish that $\tilde{I}(x,y)$ is lower semi-continuous (l.s.c.), we proceed as in the proof of the contraction principle in large deviation theory, see, e.g., [5]: The function $\omega \mapsto (-s(\omega) + \omega(E_\Phi))$ is l.s.c. and the set $\{\omega \in \mathcal{S}_{\mathrm{erg}}, \omega(X) = x,\, \omega(Y) = y\}$ is compact by the continuity of $\omega \mapsto (\omega(X), \omega(Y))$ (compactness and continuity with respect to the weak*-topology). Therefore, the infimum is attained and we can deduce that

$$\{x, y \,|\, \tilde{I}(x,y) \le a\} = F(\{\omega \in \mathcal{S}_{\mathrm{erg}} | -s(\omega) + \omega(E_\Phi) \le a\}) \tag{3.9}$$

where $F : \omega \mapsto (\omega(X), \omega(Y))$. The level set on the left-hand side is closed and hence $\tilde{I}$ is l.s.c.

By using the infinite-volume Gibbs variational principle [12, 20], the Legendre–Fenchel transform of $\tilde{I}$ reads

$$\begin{aligned}\sup_{(x,y)\in\mathbb{R}^2}(ux+vy-\tilde{I}(x,y)) &= \sup_{\omega\in\mathcal{S}_{\mathrm{erg}}}(s(\omega)-\omega(E_\Phi)+u\,\omega(X)+v\,\omega(Y))\\ &= p(u,v).\end{aligned} \tag{3.10}$$

The equality $I=\tilde{I}$ then follows by the involution property of the Legendre–Fenchel transform on the set of convex lower-semicontinuous functions, see, e.g., [20]. □

Independence of boundary conditions. Observe that both Theorems 3.1 and 3.2 have been formulated for the finite volume Gibbs states with open boundary conditions. It is however easy to check that this choice is not essential and other equivalent formulations can be obtained. Indeed, by the standard log-trace inequality,

$$|\log\mathrm{Tr}_\Lambda(e^{-\beta H_\Lambda+W_\Lambda+|\Lambda|\,G(\bar{X}_\Lambda,\bar{Y}_\Lambda)})-\log\mathrm{Tr}_\Lambda(e^{-\beta H_\Lambda+|\Lambda|\,G(\bar{X}_\Lambda,\bar{Y}_\Lambda)})|\leq\|W_\Lambda\| \tag{3.11}$$

and hence if one chooses W_Λ such that $\lim_{\Lambda\nearrow\mathbb{Z}^d}\|W_\Lambda\|/|\Lambda|=0$, then we can replace $-\beta H_\Lambda$ by $-\beta H_\Lambda+W_\Lambda$ in Theorems 3.1 and 3.2.

Finite-range restrictions. It is obvious that our paper contains some restrictions that are not essential. In particular, by standard estimates (in particular, those used to prove the existence of the pressure, see, e.g., [20]) one can relax the finite-range conditions on the interaction Φ to the condition that

$$\sum_{A\ni 0}\frac{\|\Phi_A\|}{|A|}<\infty, \tag{3.12}$$

and similarly for the local observables X,Y. Moreover, it is not necessary that G is a non-commutative polynomial. Starting from (3.11), one checks that it suffices that G can be approximated in operator norm by non-commutative polynomials.

4. Approximation by Ergodic States

In this section, we describe a construction that is the main ingredient of our proofs, as well as of those in [10, 17]. This construction will be used in Secs. 6 and 7.

Let V be a hypercube centered at the origin, i.e. $V=[-L,L]^d$ for some $L>1$ and let

$$\partial V := \{i\in V\,|\,\exists i'\in\mathbb{Z}^d\backslash V \text{ such that } i,i' \text{ are nearest neighbors}\} \tag{4.1}$$

We write

$$\mathbb{Z}^d/V=((2L+1)\mathbb{Z})^d \tag{4.2}$$

to denote the "block lattice" whose points can be thought of as translates of V. In other words, $\mathbb{Z}^d=\cup_{i\in\mathbb{Z}^d/V}V+i$. Consider a state μ_V on $\mathcal{B}_V$.

We aim to build an infinite-volume ergodic state out of μ_V. First, we define the block product state

$$\tilde{\mu} := \bigotimes_{\mathbb{Z}^d/V} \mu_V. \tag{4.3}$$

We define also the translation-average of $\tilde{\mu}$,

$$\bar{\mu} := \frac{1}{|V|}\sum_{j\in V} \tilde{\mu}\circ\tau_j. \tag{4.4}$$

We can now check the following properties:

- We have the exact equality of entropies

$$s(\bar{\mu}) = s(\tilde{\mu}) = \frac{1}{|V|}S(\mu_V). \tag{4.5}$$

  This follows from the affinity of the entropy in infinite-volume. A remark is in order: *A priori*, the infinite-volume entropy is defined for translation-invariant states, whereas $\tilde{\mu}$ is only periodic. However, one easily sees that the entropy can still be defined, e.g. be viewing $\tilde{\mu}$ as a translation-invariant state on the block lattice $\mathbb{Z}^d/V$, and correcting the definition by dividing by $|V|$.
- The state $\bar{\mu}$ is ergodic. This follows, for example, from an explicit calculation that is presented in [10]. Note however that $\bar{\mu}$ is in general not ergodic with respect to the translations over the sublattice $\mathbb{Z}^d/V = ((2L+1)\mathbb{Z})^d$. This phenomenon (though in a slightly different setting) is commented upon in [20] (the end of Sec. III.5).
- The state $\bar{\mu}$ is a good approximation of μ_V for observables which are empirical averages, provided V is large. Consider the local observable X as in Sec. 2.1. A translate $\tau_j X$ can lie inside a translate of V, i.e. $\operatorname{Supp}\tau_j X \subset V+i$ for some $i\in\mathbb{Z}^d/V$, or it can lie on the boundary between two translates of V. The difference between $\bar{\mu}(X)=\bar{\mu}(\bar{X})$ and $\mu_V(\bar{X}_V)$ clearly stems from those translates where X lies on a boundary, and the fraction of such translates is bounded by

$$|\operatorname{Supp} X| \times \frac{|\partial V|}{|V|}. \tag{4.6}$$

  Hence

$$|\bar{\mu}(\bar{X}) - \mu_V(\bar{X}_V)| \le \|X\| |\operatorname{Supp} X| \times \frac{|\partial V|}{|V|}. \tag{4.7}$$

5. The Lower Bound

In this section, we prove the following lower bound.

Lemma 5.1. *Recall $Z^G_\Lambda(\Phi)$ as defined in (3.1). Then*

$$\liminf_{\Lambda\nearrow\mathbb{Z}^d} \frac{1}{|\Lambda|}\log Z^G_\Lambda(\Phi) \ge \sup_{\omega\in\mathcal{S}_{\mathrm{erg}}} ((g(\omega(X),\omega(Y)) + s(\omega) - \omega(E_\Phi)) \tag{5.1}$$

where all symbols have the same meaning as in Sec. 3.

Proof. Consider a state $\omega \in \mathcal{S}_{\mathrm{erg}}$. We show that

$$\liminf_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log Z_\Lambda^G(\Phi) \geq g(\omega(X), \omega(Y)) + s(\omega) - \omega(E_\Phi). \tag{5.2}$$

Consider, for each volume Λ, the restriction $\omega_\Lambda := \omega\big|_{\mathcal{B}_\Lambda}$. By the finite-volume variational principle (see, e.g., [2, Proposition 6.2.22]),

$$\frac{1}{|\Lambda|} \log Z_\Lambda^G(\Phi) \geq \omega_\Lambda(G(\bar{X}_\Lambda, \bar{Y}_\Lambda)) + \frac{1}{|\Lambda|} S(\omega_\Lambda) - \frac{1}{|\Lambda|} \omega_\Lambda(H_\Lambda). \tag{5.3}$$

The following convergence properties apply with $\Lambda \nearrow \mathbb{Z}^d$ in the sense of Van Hove:

(1) $$\omega_\Lambda(G(\bar{X}_\Lambda, \bar{Y}_\Lambda)) = \omega(G(\bar{X}_\Lambda, \bar{Y}_\Lambda)) \to g(\omega(X), \omega(Y)), \tag{5.4}$$

(2) $$\frac{1}{|\Lambda|} S(\omega_\Lambda) \to s(\omega), \tag{5.5}$$

(3) $$\frac{1}{|\Lambda|} \omega(H_\Lambda) \to \omega(E_\Phi). \tag{5.6}$$

The relation (5.6) is obvious from the finite range condition on Φ, see Sec. 2.1. The convergence (5.5) is the definition of the mean entropy s. Finally, (5.4) follows from the ergodicity of ω as explained in Sec. 2.3.

The relation (5.2) now follows immediately, since one can repeat the above construction for any ergodic state ω. □

6. The Upper Bound

6.1. *Reduction to product states*

In this section, we outline how to approximate

$$\frac{1}{|\Lambda|} \log Z_\Lambda^G(\Phi) \tag{6.1}$$

by a similar expression involving the partition function of a block-product state. Fix a hypercube $V = [-L, L]^d$ and cover the lattice with its translates, as explained in Sec. 4. From now on, Λ is chosen such that it is a multiple of V. One can easily adopt the arguments such as to cover the case where Λ tends to infinity in the sense of Van Hove (as one has to do as well in the proof of the existence of the pressure for local interactions, see [12]).

Define the observables

$$H_\Lambda^V \equiv H_\Lambda^{\Phi,V}, \quad \bar{X}_\Lambda^V, \quad \bar{Y}_\Lambda^V \tag{6.2}$$

by cutting all terms that connect any two translates of V, i.e.

$$\bar{X}_\Lambda^V := \frac{1}{|\Lambda|} \sum_{\substack{j \in \Lambda \\ \exists i \in \mathbb{Z}^d/V : \operatorname{Supp} \tau_j X \subset V + i}} \tau_j X, \tag{6.3}$$

and analogously for H_Λ^V and $\bar{Y}_\Lambda^V$. One can say that these observables with superscript V are one-block observables with the blocks being translates of V. One easily derives that

$$\|\bar{X}_\Lambda^V - \bar{X}_\Lambda\| \le \|X\||\mathrm{Supp}\,X|\frac{|\partial V|}{|V|}, \quad \|H_\Lambda^V - H_\Lambda\| \le r(\Phi)|\Lambda|\frac{|\partial V|}{|V|} \tag{6.4}$$

with the number $r(\Phi)$ as defined in Sec. 2.1.

Using the log-trace inequality, we bound

$$\frac{1}{|\Lambda|}\log \mathrm{Tr}_\Lambda(e^{-H_\Lambda+|\Lambda|\,G(\bar{X}_\Lambda,\bar{Y}_\Lambda)}) - \frac{1}{|\Lambda|}\log \mathrm{Tr}_\Lambda(e^{-H_\Lambda^V+|\Lambda|G(\bar{X}_\Lambda^V,\bar{Y}_\Lambda^V)}) \tag{6.5}$$

as follows

$$\begin{aligned}(6.5) &\le \frac{1}{|\Lambda|}\|H_\Lambda - H_\Lambda^V\| + \|G(\bar{X}_\Lambda,\bar{Y}_\Lambda) - G(\bar{X}_\Lambda^V,\bar{Y}_\Lambda^V)\|\\ &\le (r(\Phi) + C_g(\|X\||\mathrm{Supp}\,X| + \|Y\||\mathrm{Supp}\,Y|))\frac{|\partial V|}{|V|}\end{aligned}$$

where C_g is constant depending on the function G. The second term of (6.5) is clearly the pressure of a product state with mean field interaction. We will find an upper bound for this pressure by slightly extending the treatment of Petz *et al.* in [17]. We prove an "extended PRV"-lemma, Lemma 6.1 in the next section.

6.2. *The extended Petz–Raggio–Verbeure upper bound*

In this section, we outline the bound from above on the quantity

$$\frac{1}{|\Lambda|}\log \mathrm{Tr}_\Lambda(e^{-H_\Lambda^V+|\Lambda|G(\bar{X}_\Lambda^V,\bar{Y}_\Lambda^V)}) \tag{6.6}$$

that appeared in (6.5).

To do this, let us make the setting slightly more abstract. Consider the lattice $\mathbb{Z}^d$ with the one-site Hilbert space $\mathcal{G}$ given by

$$\mathcal{G} := \bigotimes_V \mathcal{H}. \tag{6.7}$$

In words, $\mathbb{Z}^d$ should be thought of as the block lattice $\mathbb{Z}^d/V$. Let D, A, B be one-site observable on the new lattice, i.e. D, A, B are Hermitian operators on $\mathcal{G}$. The extended PRV (Petz–Raggio–Verbeure) states that

Lemma 6.1 (Extended PRV). *Let all symbols have the same meaning as in Secs.* 2.1–2.3, *except that the one-site Hilbert space is changed from $\mathcal{H}$ to $\mathcal{G}$. Then*

$$\limsup_{\Lambda\nearrow\mathbb{Z}^d}\frac{1}{|\Lambda|}\log \mathrm{Tr}_\Lambda(e^{-D_\Lambda+|\Lambda|G(\bar{A}_\Lambda,\bar{B}_\Lambda)}) \le \sup_{\omega\in\mathcal{S}_{\mathrm{sym}}}(\omega(G(\bar{A},\bar{B})) + s(\omega) - \omega(D)). \tag{6.8}$$

In particular $\omega(G(\bar{A},\bar{B}))$ defined as (2.17) *exists.*

To appreciate the similarity between (6.8) and (3.6), one should realize that D is a local energy operator, as E_Ψ in (3.6). The proof of this lemma in the case that $A = B$ is in the original paper [17]. The proof for the more general case is presented in Sec. 7. Of course, one can prove that the right-hand side of (6.8) is also a lower bound: it suffices to copy Sec. 5.

By the Størmer theorem, see (2.14), each symmetric state ω on $\mathfrak{U}$ can be written as the barycenter of a regulary probability measure on the product states, and since all terms on the right-hand side of (6.8) are affine and upper semicontiuous functions of ω, it follows that the sup can be restricted to product states (see [17] for the fine details of this argument). Since, moreover, all product states are ergodic, we can replace $\omega(G(\bar{A},\bar{B}))$ by $g(\omega(A),\omega(A))$. Hence, Lemma 6.1 implies that

$$\limsup_{\Lambda\nearrow\mathbb{Z}^d}\frac{1}{|\Lambda|}\log\operatorname{Tr}_\Lambda(e^{-D_\Lambda+|\Lambda|G(\bar{A}_\Lambda,\bar{B}_\Lambda)})\leq\sup_{\omega\,\text{prod.}}(g(\omega(A),\omega(B))+s(\omega)-\omega(D)). \tag{6.9}$$

6.2.1. *From the extended PRV to the upper bound*

Next, we use (6.9) to formulate an upper bound on the quantity

$$\frac{1}{|\Lambda|}\operatorname{Tr}_\Lambda(e^{-H_\Lambda^V+|\Lambda|G(\bar{X}_\Lambda^V,\bar{Y}_\Lambda^V)}) \tag{6.10}$$

for Λ a multiple of V. This means that we have to recall that the lattice sites in (6.9) are in fact blocks. We write $\Lambda^*:=\Lambda/V$ and choose

$$\begin{aligned}D&:=H_V\\A&:=\bar{X}_V\\B&:=\bar{Y}_V.\end{aligned}$$

Then, by the extended PRV,

$$\begin{aligned}(6.10)&\leq\sup_{\omega\,\text{prod. on}\,\mathcal{B}(\Lambda^*)}\left(g(\omega(A),\omega(B))+\frac{1}{|V|}s^*(\omega)-\frac{1}{|V|}\omega(D)\right)\\&=\sup_{\omega_V\,\text{on}\,\mathcal{B}_V}\left(G(\omega_V(\bar{X}_V),\omega_V(\bar{Y}_V))+\frac{1}{|V|}S(\omega_V)-\frac{1}{|V|}\omega_V(H_V)\right)\end{aligned}$$

where s^* indicates that this is the entropy density on the block lattice Λ^*, hence it should be divided by $|V|$ to obtain the density on Λ. Now, let $\tilde{\omega}$ be the infinite-volume state obtained by taking a block-product over states ω_V and let $\bar{\omega}$ be its "translation-average", as in Sec. 4. By the conclusions of Sec. 4, it follows that $\bar{\omega}$ is ergodic and $s(\bar{\omega})=S(\omega_V)$. Also, we see that

$$\begin{aligned}|\omega_V(\bar{X}_V)-\bar{\omega}(X)|&\leq\|X\||\operatorname{Supp}X|\frac{|\partial V|}{|V|}\\\frac{1}{|V|}|\omega_V(H_V)-\bar{\omega}(E_\Phi)|&\leq r(\Phi)\frac{|\partial V|}{|V|}\end{aligned}$$

and analogously for $\bar{Y}_V$. Consequently, we obtain

$$(6.10)\leq\sup_{\omega\in\mathcal{S}_{\text{erg}}}(g(\omega(X),\omega(Y))+s(\omega)-\omega(E_\Phi))+O\left(\frac{|\partial V|}{|V|}\right),\quad V\nearrow\mathbb{Z}^d$$

which proves the upper bound for Theorem 3.2, since the $O(\frac{|\partial V|}{|V|})$-term can be made arbitrarily small by increasing V.

7. Proof of Lemma 6.1

Let the state μ_Λ on $\mathcal{B}_\Lambda$ be given by

$$\mu_\Lambda(\,\cdot\,) = \frac{1}{Z_\Lambda^G(D)} \operatorname{Tr}_\Lambda(e^{-D_\Lambda + |\Lambda| G(\bar{A}_\Lambda, \bar{B}_\Lambda)}\ \cdot)$$

with

$$Z_\Lambda^G(D) := \operatorname{Tr}_\Lambda(e^{-D_\Lambda + |\Lambda| G(\bar{A}_\Lambda, \bar{B}_\Lambda)}).$$

Naturally, μ_Λ is the finite-volume Gibbs state that saturates the variational principle, i.e.

$$\begin{aligned} \frac{1}{|\Lambda|} \log Z_\Lambda^G(D) &= \sup_{\omega_\Lambda \text{ on } \mathcal{B}_\Lambda} \left(\omega_\Lambda(G(\bar{A}_\Lambda, \bar{B}_\Lambda)) + \frac{1}{|\Lambda|} S(\omega_\Lambda) - \omega_\Lambda(D) \right) \\ &= \mu_\Lambda(G(\bar{A}_\Lambda, \bar{B}_\Lambda)) + \frac{1}{|\Lambda|} S(\mu_\Lambda) - \mu_\Lambda(D). \end{aligned} \tag{7.1}$$

Our strategy is to attain the "entropy" and "energy" of the state μ_Λ via ergodic states. For definiteness, we assume that G is of the form

$$G(\bar{A}_\Lambda, \bar{B}_\Lambda) := [\bar{A}_\Lambda]^k [\bar{B}_\Lambda]^l \quad \text{for some integers } k, l,$$

(which, strictly speaking, is not allowed since $G(\bar{A}_\Lambda, \bar{B}_\Lambda)$ has to be a self-adjoint operator, but this does not matter for the argument in this section). The general case follows by the same argument.

We apply the construction in Sec. 4 to μ_Λ, thus obtaining infinite-volume states $\tilde{\mu}$ and $\bar{\mu}$. Since we will repeat the construction for different Λ, we indicate the Λ-dependence in $\tilde{\mu}^{\{\Lambda\}}$ and $\bar{\mu}^{\{\Lambda\}}$, but remembering that these are states on the infinite lattice. They satisfy

$$s(\bar{\mu}^{\{\Lambda\}}) = \frac{1}{|\Lambda|} S(\mu_\Lambda). \tag{7.2}$$

We have also established in Sec. 4 that $\bar{\mu}^{\{\Lambda\}}$ is ergodic and that the states $\bar{\mu}^{\{\Lambda\}}$ and $\tilde{\mu}^{\{\Lambda\}}$ approximate μ_Λ for observables which are empirical averages. However, we cannot conclude yet that they have comparable values for $G(\bar{A}, \bar{B})$, except in the case where G is linear. Essentially, such a comparison is achieved next by using the fact that μ_Λ is symmetric.

Choose a sequence of volumes Λ_n such that along that sequence the right-hand side of (7.1) converges. We assume that $\bar{\mu}^{\Lambda_n}$ has a weak$*$-limit, as $n \nearrow \infty$, which can always be achieved (by the weak$*$-compactness) by restricting to a subsequence of Λ_n. We call this limit μ. By construction, it is a symmetric state.

Energy estimate. Since $\bar{\mu}^{\Lambda_n} \to \mu$, in the weak$*$-topology, and $\bar{\mu}^{\Lambda_n}(D) = \mu_{\Lambda_n}(D)$, we have

$$\mu_{\Lambda_n}(D) \to \mu(D). \tag{7.3}$$

G-estimates. Using the symmetry of the state μ_Λ, we estimate

$$\begin{aligned} &|\mu_\Lambda(G(\bar{A}_\Lambda, \bar{B}_\Lambda)) - \mu_\Lambda(\otimes^k A \otimes^l B)| \\ &\quad \le \max\left(\|A\|, \|B\|\right)^{k+l} \left(\frac{(k+l)^2}{|\Lambda|} + O\left(\frac{c(k,l)}{|\Lambda|^2}\right)\right), \quad |\Lambda| \nearrow \infty \end{aligned} \tag{7.4}$$

where the tensor products

$$\otimes^k A \otimes^l B := \underbrace{A \otimes \cdots \otimes A}_{k \text{ copies}} \otimes \underbrace{B \otimes \cdots \otimes B}_{l \text{ copies}} \tag{7.5}$$

denote that all one-site operators are placed on different sites. Since μ_Λ is symmetric, we need not specify on *which* sites. The error term of order $1/|\Lambda|$ comes from those terms in the expansion of the monomial containing a product of $k+l$ one-site operators but only involving $k+l-1$ sites. Since μ is symmetric, we obtain analogously that

$$\mu(G(\bar{A}, \bar{B})) = \mu(\otimes^k A \otimes^l B). \tag{7.6}$$

In particular, the left-hand side is well-defined. Hence, by combining (7.4) and (7.6), we obtain

$$\mu_{\Lambda_n}(G(\bar{A}_{\Lambda_n}, \bar{B}_{\Lambda_n})) \to \mu(G(\bar{A}, \bar{B})). \tag{7.7}$$

For a more general non-commutative polynomial G as defined in Sec. 2.2 (not necessarily a monomial), the convergence (7.7) follows easily since $G(\bar{A}_{\Lambda_n}, \bar{B}_{\Lambda_n})$ can be approximated in operator norm by polynomials.

Entropy estimates. As established in Sec. 4, we have

$$\frac{1}{|\Lambda|} S(\mu_\Lambda) = s(\bar{\mu}^{\{\Lambda\}}), \quad \text{for all } \Lambda. \tag{7.8}$$

By the upper semi-continuity of the infinite-volume entropy and the convergence $\bar{\mu}^{\Lambda_n} \to \mu$, we get that

$$\limsup_{n \nearrow \infty} s(\bar{\mu}^{\{\Lambda_n\}}) \le s(\mu). \tag{7.9}$$

Hence

$$\lim_{n \nearrow \infty} \frac{1}{|\Lambda_n|} S(\mu_{\Lambda_n}) \le s(\mu). \tag{7.10}$$

By combining the convergence results (7.3), (7.7) and (7.10), we have proven that there is a symmetric state μ such that the right-hand side of (6.8) with $\omega \equiv \mu$ is larger than a given limit point of the right-hand side of (7.1). Since the construction can be repeated for any limit point, this concludes the proof of Lemma 6.1.

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Appendix. Proof of Lemma 2.2

To prove Lemma 2.2, it is convenient to introduce an extended framework: Let π_ω be the cyclic GNS-representation associated to the state ω, $\mathfrak{H}_\omega$ the associated Hilbert space and $\psi \in \mathfrak{H}_\omega$ the representant of the state ω, i.e.

$$\omega(A) = \langle \psi, \pi_\omega(A)\psi\rangle_{\mathfrak{H}_\omega}, \quad A \in \mathfrak{U}. \tag{A.1}$$

The set $\pi_\omega(\mathfrak{U})$ is a subalgebra of $\mathcal{B}(\mathfrak{H}_\omega)$. Let $U_j, \in \mathbb{Z}^d$ be the unitary representation of the translation group induced on $\pi_\omega(\mathfrak{U})$, i.e.

$$U_j \pi_\omega(A) U_j^* = \pi_\omega(\tau_j A). \tag{A.2}$$

Ergodicity of ω implies (see, e.g., the proof of [20, Theorem III.1.8]) that

$$\frac{1}{|\Lambda|}\sum_{j\in\Lambda} U_j \xrightarrow[\Lambda\nearrow\mathbb{Z}^d]{\text{strongly}} P_\psi \tag{A.3}$$

where P_ψ is the one-dimensional orthogonal projector associated to the vector ψ, and $\Lambda \nearrow \mathbb{Z}^d$ in the sense of Van Hove. Using (A.3) and the translation-invariance $U_j\psi = \psi$, one calculates

$$\begin{aligned} \pi(\bar{X}_\Lambda)\pi(\bar{Y}_\Lambda)\psi &= \frac{1}{|\Lambda|^2}\sum_{j,j'\in\Lambda} U_j \pi(X) U_{j'-j}\pi(Y) U_{-j'}\psi \\ &\overrightarrow{\Lambda\nearrow\mathbb{Z}^d}\ P_\psi \pi(X) P_\psi \pi(Y)\psi = \omega(X)\omega(Y)\psi \end{aligned}$$

for local observables $X, Y \in \mathfrak{U}$. Taking the scalar product with ψ, we conclude that $\omega(\bar{X}_\Lambda \bar{Y}_\Lambda) \to \omega(X)\omega(Y)$. The same argument works for all polynomials in $\bar{X}_\Lambda, \bar{Y}_\Lambda$, thus proving Lemma 2.2. Finally, we remark that one can also construct the operators $\bar{X}, \bar{Y}$ as weak$*$-limits of $\bar{X}_\Lambda, \bar{Y}_\Lambda$, as $\Lambda \nearrow \mathbb{Z}^d$ (these weak$*$-limits are simply multiples of identity: $\omega(X)1, \omega(Y)1$). This is however not necessary for our results.

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