Properties of thermal states: locality of temperature, decay of correlations, and more

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We review several properties of thermal states of spin Hamiltonians with short range interactions. In particular, we focus on those aspects in which the application of tools coming from quantum information theory has been specially successful in the recent years. This comprises the study of the correlations at finite and zero temperature, the stability against distant and/or weak perturbations, the locality of temperature and their classical simulatability. For the case of states with a finite correlation length, we overview the results on their energy distribution and the equivalence of the canonical and microcanonical ensemble.

I. INTRODUCTION

Thermal or Gibbs states are arguably the most relevant class of states in nature. They appear to have many very different unique properties. On one hand, they provide an efficient description of the equilibrium state for most systems (see [1, Chapter 17] and Ref. [2] for a detailed review). Jaynes gave a justification of this observation by means of the principle of maximum entropy [3, 4]. For a given energy, the thermal state is the one that maximizes the von Neumann entropy. This is in fact the reason why they minimize the free energy potential.

At the same time, in the context of extracting work from closed systems by means of unitary transformations, thermal states appear as the only ones that are completely passive states [5]. That is, for any other passive state [6], i.e. a state whose (average) energy cannot be lowered by applying a unitary transformation, it is always possible to form an active state by joining sufficiently many copies. Note that this property is crucial for establishing both a resource theory of thermodynamics and a consistent zero-th law (see the book chapters [1, Chapters 25] and [7]).

Last but not least, if one accepts that the equilibrium population of a configuration should only be a function of its energy, the canonical ensemble becomes the single probability distribution that allows for a free choice of the energy origin, or in other words, that is invariant under energy shifts. More explicitly, any other relation between populations and energy would imply that observers with different energy origins would observe different equilibrium states. The proof of this statement is a good exercise.

In this chapter, we study of the properties of thermal states for a class of Hamiltonians highly relevant in condensed matter physics: the spin lattice Hamiltonians with short range interactions. We particularly focus on results where the application of tools coming from quantum information theory has been particularly successful in the recent years.

A first issue where quantum information tools have been helpful is in the rigorous proof of long-standing conjectures concerning the correlations of many-body systems. The most paradigmatic example is the proof that unique ground states of gapped Hamiltonians have an exponential decay of the correlations [8, 9]. In Section III we overview the main results on the scaling of the correlations for both thermal states and absolute zero temperature states. The understanding of the correlations of many-body systems is particularly relevant since they are a signature of phase transitions and critical phenomena [10, 11]. Furthermore, they are also related to the stability of thermal states, that is, to the robustness of thermal states against distant and/or weak Hamiltonian perturbations [12].

The stability of thermal states is actually crucial for understanding to what extent temperature can be assigned locally in a system [12, 13]. For weakly interacting systems temperature is an intensive quantity, in the sense that every subsystem is in a thermal state with the temperature identical to the global one. However, when interactions between subsystems are not negligible, this property does no longer hold, as can be the case for quantum systems [14, 15]. Further steps to circumvent the problem of assigning temperature locally to a subsystem were made in Refs. [16, 17], where it was shown that it is sufficient to extend the subsystem by a boundary region that, when traced out, disregards the correlations and the boundary effects. If the size of such a boundary region is independent of the total system size, temperature can still be said to be local. In Ref. [12] it is shown that the thickness of the boundary region is determined by the decay of a generalized covariance, which captures the response in a local operator of perturbing a thermal state and ultimately at what length scales temperature can be defined. In other words, the clustering of the generalized covariance allows for a local definition of temperature. This issue is particularly relevant in the book

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chapter [18], where the problem of local thermometry is considered.

Another feature of the thermal states that exhibit a clustering of correlations is that they can be efficiently classically represented by so-called tensor network states [19]. The simulation of quantum many body systems by classical means, and more specifically by using tensor network states, has been one of the most fruitful topics in the interplay between condensed-matter physics and quantum information. Tensor networks have been shown to satisfactorily describe locally entangled states in one and two spatial dimensions and even systems at criticality [20]. Applications of thermal states with exponentially decaying correlations are presented in Section IV.

In Section V, we focus on the study of the energy distribution of states not necessarily thermal but with a finite correlation length. In particular, it can be shown that for large system sizes the energy distribution of a state with a finite correlation length has an energy distribution that tends to a Gaussian whose standard deviation scales with a finite correlation length has an energy distribution.

For a boundary we have \( \partial \{2, 3, 4\} = \{2, 4\} \). Moreover, \( \text{dist}(h_{1, 2}, h_{6, 7}) = 6 - 2 = 4 \).

We denote the thermal state, or Gibbs state, of a Hamiltonian \( H \) at inverse temperature \( \beta \) by

\[
g(\beta) := \frac{e^{-\beta H}}{Z(\beta)},
\]

with \( Z(\beta) := \text{Tr}(e^{-\beta H}) \) being the partition function. If we mean the thermal state or partition function of a different Hamiltonian \( H' \), we write \( g(H')(\beta) \) or \( Z(H')(\beta) \).

We measure correlations by the (generalized) covariance that we define for any two operators \( A \) and \( A' \), full-rank quantum state \( \rho \), and parameter \( \tau \in [0, 1] \) as

\[
\text{cov}_{\tau}(A, A') := \text{Tr}(\rho^\tau A \rho^{1-\tau} A') - \text{Tr}(\rho A) \text{Tr}(\rho A').
\]

This quantity is closely related to the Duhamel two-point function, which is defined as the average \( \int_0^1 d\tau \text{Tr}(\rho^\tau A \rho^{1-\tau} A') \) (see, e.g., [23, Section 2]). The usual covariance, denoted by \( \text{cov}(A, A') \), is obtained by setting \( \rho^\tau = \rho \) and \( \rho^{1-\tau} = 1 \), see also [12, Section IV.A].

It is interesting to point out that the clustering of the standard covariance implies the clustering of the Duhamel two-point function [23, Theorem 2.1]. In this case, we mean by clustering that the covariance tends to zero in the limit of the spatial distance between the non-trivial support of the operators \( A \) and \( A' \) tends to infinity. However, given a state \( \rho \) and two observables \( A \) and \( A' \), the generalized covariance as a function of \( \tau \) is not monotonic and can have zeros and saddle points.

Let us finally introduce the relative entropy between two quantum states \( \rho \) and \( \sigma \), which is defined as

\[
S(\rho||\sigma) := -\text{Tr}(\rho \log_2(\sigma)) - S(\rho),
\]
where $S(\rho) := -\text{Tr}[\rho \log_2(\rho)]$ is the von Neumann entropy. The relative entropy provides a notion of non-symmetric distance between states, and can be operationally interpreted as the physical distinguishability from many copies [24]. The relative entropy is closely related to the free energy when its second argument $\sigma$ is a thermal state,

$$F(\rho) - F(g(\beta)) = \frac{1}{\beta} S(\rho|g(\beta)), \tag{5}$$

where $F(\rho, H) := \text{Tr}[(\rho H) - \beta^{-1}S(\rho)]$ is the out of equilibrium free energy. In a similar way, the mutual information of a bipartite state $\rho$ can also be written in terms of the relative entropy

$$I(A : B)_\rho = S(\rho|\rho_A \otimes \rho_B). \tag{6}$$

Recall that the mutual information, defined as $I(A : B)_\rho := S(\rho_A) + S(\rho_B) - S(\rho)$, is a measure of the total correlations between the parties $A$ and $B$ [25].

III. CLUSTERING OF CORRELATIONS

In quantum lattice models with local Hamiltonians, a relevant class of observables are the local ones, that is, operators that only have non-trivial support on a few connected sites. However, local operators cannot witness global properties of the system such as entanglement, correlations or long range order. The simplest observables that can reveal this type of features are the two-point correlation functions or, as they have been introduced in the former section, the covariance. In condensed-matter physics, the scaling of the covariance with the distance between the two “points” is an important correlations measure. In this section, we review the current understanding on the sorts of scalings that the covariance of thermal states and zero temperature states can exhibit.

A. High temperature states

Bounding correlations in thermal spin systems has a long tradition in theoretical and mathematical physics; see e.g. Ref. [26] classical systems, [27] for quantum gases (translation-invariant Hamiltonians in the continuum), and Refs. [28–30] cubic lattices. Here, we review a general result for finite dimensional systems.

Any graph that is a regular lattice has an associated (cell or lattice animal) growth constant $\alpha \in \mathbb{R}_+$, which captures the local connectivity of a lattice [31, 32]. For instance, for lattices in $D$ spatial dimensions, $\alpha \leq 2D \exp(1)$ [32, Lemma 2].

The following theorem provides a universal upper bound to all critical temperatures that only depends on the growth constant $\alpha$.

Theorem 1 (High temperatures [12, Theorem 2]). For a graph $(V, E)$ with growth constant $\alpha$ define the constant (critical inverse temperature)

$$\beta^* := \ln\left[(1 + \sqrt{1 + 4/\alpha})/2\right]/(2J) \tag{7}$$

and function $\xi$ (correlation length) by

$$\xi(\beta) := \left|\ln[\alpha e^{2/\beta}J(e^{2/\beta}J - 1)]\right|^{-1}. \tag{8}$$

Then, a thermal state $\rho$ of any Hamiltonian with interaction graph $(V, E)$ and local interaction strength $J$ satisfies the following: for every $|\beta| < \beta^*$, parameter $\tau \in [0, 1]$, and every two operators $A$ and $B$

$$|\text{cov}_{\rho}^\tau(A, B)| \leq \frac{4\alpha}{\ln(3)(1 - e^{-1/\xi(\beta)\beta})} e^{-\beta\text{dist}(A, B)/\xi(\beta)}, \tag{9}$$

disregarding some minimal distance $L_0$ (given in [12, Eq. (50)]) and with parameter $\alpha := ||A|| ||B|| \min\{|\partial A|, |\partial B|\}$.

This theorem guarantees that below an inverse universal critical temperature $\beta^*$ correlations always decay with a correlation length at most $\xi(\beta)$. The inverse critical temperature $\beta^*$ and correlation length $\xi$ are universal bounds to the corresponding actual physical quantities.

For the proof of Theorem 1, four weighted copies of the system $V$ are considered and a cluster expansion analysis from Hastings [33] is tightened for this particular case. Originally, Hastings used this cluster expansion to show that high temperature thermal states on spin lattices can be approximated by so-called MPOs; see also Section IV C on classical simulatability below.

B. Ground states of gapped Hamiltonians

The following theorem, first proved by Hastings, Koma, Nachtergaele, and Sims [8, 9], confirmed a longstanding conjecture in condensed-matter physics, that gapped Hamiltonian systems have exponentially clustering correlations in the ground state. A gapped Hamiltonian is a Hamiltonian whose gap, i.e., the energy difference between the ground state and the first excited state (or eigenspace), is lower bounded by a constant in the thermodynamic limit. The proof of the theorem is based on Lieb-Robinson bounds which provide a bound on the speed of propagation of correlation under Hamiltonian evolution. There is a constant speed limit that only depends on the maximum number of lattice nearest neighbors and the interaction strength and is called Lieb-Robinson speed, see Ref. [34] for a review on that topic.

Theorem 2 (Unique ground states [35, Theorem 4.1]). Let $H$ be a local Hamiltonian with interaction graph $(V, E)$, a unique ground state $\psi$, and a spectral gap $\Delta E > 0$. Then, for all observables $A$ and $B$

$$|\text{cov}_{\psi}(A, B)| \leq C a e^{-\beta \text{dist}(A, B)}, \tag{10}$$
where \( a := \|A\|\|B\|_\infty \min\{\|\partial A\|,\|\partial B\|\} \), the constant \( C \) depends on \( \Delta E \) and the local lattice geometry, and the constant \( \mu \) on \( \Delta E \) and the Lieb-Robinson speed.

This theorem tells us that correlations in ground states of gapped Hamiltonians decay with a correlation length that is bounded in terms of the spectral energy gap above the ground state.

It is interesting to point out that one dimensional systems in a pure state with exponentially decaying correlations obey an area law for the entanglement entropy [36], that is, the entropy of the reduced state of a subregion grows like its boundary and not like its volume [37]. The same statement remains open in higher dimensions. Theorem 2 together with Ref. [36] is an alternative way to see that ground-states of gapped Hamiltonians obey an area law for the entanglement entropy [38].

For the case of non-zero temperature, by inserting in Eq. (5) the thermal states of an interacting Hamiltonian \( H = H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_E + H_I \) and a non-interacting one \( H_S \otimes \mathbb{1} + \mathbb{1} \otimes H_E \) of a composite system with parts \( S \) and \( E \), one obtains

\[
I(S : E)_{\beta(g)} \leq 2 \beta \|H_I\| - S[g^S(\beta) \otimes g^E(\beta)](g(\beta))
\]

for the mutual information of \( S \) and \( E \). This equation implies an area law for the mutual information when applied on local Hamiltonians since \( \|H_I\| \) scales as the boundary between \( S \) and \( E \) [39] and the relative entropy is non-negative.

The area law for the mutual information does not contradict the fact that most energy eigenstates of non-integrable/chaotic systems away from the edges of the spectrum exhibit a volume law for the entanglement entropy [37, 40, 41]. At relatively large temperatures, when these excited states start to have non-negligible populations, their contribution to the entropy due to exhibiting a volume law is compensated by the entropy of the global state, which also exhibits a volume law for the entanglement.

C. Critical points at zero and finite temperature

We have seen that in the regime of high temperatures and for gapped Hamiltonians at absolute zero temperature the covariance decays exponentially with the distance. In the following, we review the behavior of correlations for gapless Hamiltonians at zero temperature and for arbitrary local Hamiltonians below the critical temperature (7).

1. Gapless Hamiltonians at zero temperature

If the system is gapless and no other assumption is made on the Hamiltonian, then, roughly speaking, any correlation behavior is possible. For instance, by a proper fine-tuning of the coupling constants of a nearest neighbor interacting spin-1/2 Hamiltonian, it is possible to maximally entangle spins arbitrarily far away [42]. It also remarkable that even ground-states of one dimensional translation invariant Hamiltonians with nearest neighbor interactions can exhibit a volume law for the entanglement entropy [43, 44].

However, in practice, the relevant gapless models in condensed-matter physics have ground states satisfying an area-law for the entanglement entropy with only logarithmic corrections. These logarithmic corrections are a manifestation of a power-law decay in the two-body correlations. It is useful to introduce the notion of critical system and the critical exponents. A system at zero temperature is said to be critical when the spectral gap \( \Delta \) between the energy ground state (space) and the first excited state closes in the thermodynamic limit. More explicitly, we say the system to be critical when the gap scales as

\[
\Delta \propto N^{-\nu},
\]

where \( N = |\mathcal{V}| \) is the system size and \( z \) and \( \nu \) are the critical exponents that control how fast the gap \( \Delta \) tends to zero. Actually, \( \nu \) is critical exponent that controls the divergence of the correlation length in the vicinity of the critical point,

\[
\xi \propto N^{\nu},
\]

and \( z \) the one that determines the dynamic scaling (see Ref. [10, Chapter 8]). The previous divergences are a signature of the scale invariance that the system experiences at criticality [10]. For a critical exponent \( z = 1 \) time and space correlations scale identically. This implies a further symmetry enhancement and the system becomes conformal invariant. The group of conformal transformations includes, in addition to scale transformations, translations and rotations. Such group is particularly powerful in 1+1 dimensions when we address the problem of the locality of temperature. The conformal symmetry completely determines the difference between a local expectation value of the infinite Hamiltonian and the truncated one.

2. Arbitrary systems at finite temperature

In a similar way to the ground state case, it is an open question what kind of scalings for the correlation functions of thermal states at finite can exhibit in general. The most common picture is that there exists at least a renormalization group fixed point in the space of couplings of the Hamiltonians [10, Chapter 3]. Away from the fixed point, the correlations decay exponentially. In contrast, in its vicinity, the renormalization group transformations can be linearized and some scaling laws for both the free energy and the correlation functions are obtained. In particular, the correlation length is shown to diverge as in Eq. (13).
D. Correlations and stability

Let us again assume that a quantum system is in a thermal state $g(\beta)$ w.r.t. an arbitrary Hamiltonian $H$. If we assume that a subsystem $S$ is little correlated with a disjoint subsystem $E$, say due spatial separation as sketched in Figure 1, then it is expected that a “perturbation” of the Hamiltonian on $E$ has only little effect on the state on $S$. This expectation can be rigorously confirmed and is implied by the following statement, which holds in more generality (no spin-lattice setup required).

**Theorem 3** (Perturbation formula [12, Theorem 1]). Let $H_0$ and $H$ be Hamiltonians acting on the same Hilbert space. For $s \in [0,1]$, define an interpolating Hamiltonian by $H(s) := H_0 + s(H - H_0)$ and denote its thermal state by $g_s := g[H(s)]$. Then,

$$\text{Tr}[Ag_0(\beta)] - \text{Tr}[Ag(\beta)] = \beta \int_0^1 \text{d}r \int_0^1 \text{d}s \text{ cov}^\gamma_{g_s(\beta)}(H - H_0, A)$$

for any operator $A$.

The theorem holds, in particular, for all observables $A$ supported on $S$ and a perturbation $H - H_0$ only supported on $E$. As

$$\|\Delta \rho^S\|_1 = \sup_{\|A\|=1} \text{Tr}[A \Delta \rho]$$  \hspace{1cm} (15)

for any operator $\Delta \rho$, the theorem indeed confirms the expectation developed before the theorem statement.

Note that due to the factor $\beta$ on the RHS, the perturbation formula (14) does not directly apply to ground states, as it is unclear how one can calculate the limit $\beta \to \infty$.

The proof of Theorem 3 is essentially a consequence of Duhamel’s formula, where the key was to find the right correlation measure, the averaged generalized covariance.

IV. APPLICATIONS

The understanding of the correlations of thermal states and, in particular, the exponential clustering in some regimes has several applications. We review the main ones in this section.

A. Thermal Lieb-Robinson bound

Whenever one has an explicit bound on the correlation decay in a thermal quantum system, the perturbation formula Theorem 3 yields an explicit local stability statement. Now we discuss this idea explicitly for small inverse temperature $\beta < \beta^*$, where an exponential correlation decay is guaranteed by Theorem 1. Specifically, we get back to the geometric setup sketched before Theorem 3 of a Hamiltonian $H_0$ that is perturbed on region $E$, which is spatially separated from a subsystem of interest $S$, e.g., such as sketched in Figure 1.

**Corollary 4** (Thermal Lieb-Robinson bound). Let $S, E \subset \mathcal{V}$ be subsystems that are separated by the minimal distance, $\text{dist}(S, E) \geq L_0$. Moreover, let $H$ and $H_0$ be Hamiltonians with $\text{supp}(H - H_0) \subseteq E$ and that have the same interaction graph satisfying the conditions of Theorem 1. Then, for any $|\beta| < \beta^*$,

$$\|g^S(\beta) - g^S_0(\beta)\|_1 \leq \frac{w|\beta| J}{1 - e^{-1/\xi(\beta)}} e^{-\text{dist}(S, E)/\xi(\beta)}$$ \hspace{1cm} (16)

where $g$ and $g_0$ are the thermal states of $H$ and $H_0$, respectively, $w := 4 \min\{|\partial S|, |\partial E|\} |E|/\ln(3)$, and $J$ bounds the interaction strengths of $H$, $H_0$, and $H - H_0$.

This result says that, at high temperatures, the effect on $S$ of the perturbation of $H_0$ on $E$ is exponentially suppressed in the distance between $S$ and $E$. In particular, this statement can be used to bound the error made when locally (on $S$) approximating a thermal state by the thermal state of a truncated Hamiltonian (see [12, Corollary 2] for an explicit discussion).

This bound is reminiscent of Lieb-Robinson bounds, which can be used, e.g., to rigorously bound the error made when locally (on $S$) approximating the time evolution operator of the full Hamiltonian by a truncated one.

The thermal Lieb-Robinson bound (16) motivates the following definition [21].

**Definition 5.** We say that a state $\rho$ on a spin lattice with graph $(\mathcal{V}, \mathcal{E})$ has $(\xi, z)$-exponentially decaying correlations if for any two observables $A, B$ that are normalized $(\|A\| = 1 = \|B\|)$ and have disjoint support

$$\text{cov}_\rho(A, B) \leq |\mathcal{V}| e^{-\text{dist}(A, B)/\xi}.$$ \hspace{1cm} (17)

Then Corollary 4 can be summarized as follows. Below the critical inverse temperature $\beta^*$ thermal states have $(\xi, z)$-exponentially decaying correlations.

B. Locality of temperature

Basic statistical mechanics teaches us that temperature is intensive, i.e., it is a physical quantity that can...
be measured locally and is the same throughout the system. This statement holds for non-interacting systems where the global thermal state is a tensor product of the local ones. However, in the presence of interactions the intensiveness of temperature can break down [14] and an extension of this concept is required. For this purpose, the idea of a buffer region was introduced [15, 16]. Here, one can take a “ring” $E = \{ v \in V : \text{dist}(v, S) = r \}$ around $S$, which yields a partition of the total system $V = B \cup E \cup F$ (disjoint union) where $B \subset S$ is the buffer region of $S$ and does not interact with $F$, see Figure 2. Next, we choose $H_0 := H_B + H_F$, where $H_B$ is the Hamiltonian only containing those interactions fully contained in $B$ and similarly for $H_F$. We consider $H - H_0$ as a perturbation and note that supp($H - H_0$) = $E$. As $g_{H_0} = g_{H_E} g_{H_B}$, Corollary 4 implies that the Hamiltonians $H$ and $H_B$ have approximately the same states on $S$, up to an error exponentially small in the distance $r$.

As the physical application, the approximation (18) can be used to assign a temperature to $S$ by just knowing the state of $B$. This idea extends the intensiveness of temperature to non-critical interacting quantum systems.

With respect to the critical case, in 1+1 dimensions, conformal symmetry completely dictates how correlation functions behave and how local expectation values of local observables of infinite systems differ from those taken for finite ones. Hence, conformal field theory establishes that

$$\text{Tr}[O g(\beta)] - \text{Tr}[O g(\beta, H_0)] \approx \frac{1}{r^y}$$

up to higher order terms, where $y$ is the scaling dimension of the operator $H_E$ [45, 46]. If $H_E$ is a standard Hamiltonian term, in the sense that the system is homogeneous, its leading scaling dimension is $y = 2$.

In what follows, the same idea leads to a computational application: The state on $S$ can be simulated by only calculating the state on $B$. If one wants to simulate the global thermal state then one can resort to certain tensor network approximations discussed in the next section.

C. Classical simulatability of many-body quantum systems

A naive approach for the classical simulation of many-body quantum systems requires an amount of resources (memory and time) that scales exponentially in the system size. However, in many cases, smart classical methods allow for the simulation of quantum systems by only employing polynomial resources. A powerful family of these methods for interacting quantum systems relies on so-called tensor networks, see [20] for an introduction. A key to the success of these methods is to find computationally friendly parametrizations of quantum many-body states that have limited correlations. The most prominent class of states are matrix product states (MPS), which usually represent state vectors in the Hilbert space of $n$ spins. The operator analogue of MPS are matrix product operators (MPOs), see Figure 3 for a rough definition. Practically, they can be used to (approximately) represent density matrices [47, 48].

Hastings has used a certain cluster expansion method to show that thermal spin lattice states can also be approximated by MPOs [33, Section V], see also [12, Section III.C]. After this cluster expansion method has been formalized [12] the MPO approximation was improved and made efficient by Molnár et al. [19].

For the cluster expansion one starts by expanding the exponential series of $e^{-\beta H}$ and the Hamiltonian sum (1) as

$$e^{-\beta H} = \sum_{j=0}^{\infty} \sum_{w \in \mathcal{E}^j} \frac{(-\beta)^j}{j!} h(w),$$

where $h(w) := h_{w_1} h_{w_2} \ldots h_{w_j}$. It can be made rigorous that correlations of range $L$ in the thermal state are due to those terms $h(w)$ where $w \in \mathcal{E}^j$ contains long connected regions in the graph $(V, \mathcal{E})$ of size at least $L [12, 33]$. The idea underlying the MPO approximation of the thermal state is to drop those terms in the series (20). Then one can show that the resulting operator approximates the thermal state for small inverse temperatures $\beta < 2\beta^*$ from Eq. (7) 1 and is an MPO, where the size of the single tensors is determined by $L [12, Theorem 3]. By an improved smart choice of selecting the terms in the series (20) one can algorithmically obtain an improved MPO approximation to thermal states where the size of the MPO tensors scales polynomially in the system size [19].

The efficient MPO approximation of thermal states [19] naturally has implications on the simulatability of

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1 The discrepancy of the factor of 2 in the inverse temperature bound is due to considering two copies of the system in the proof of Theorem 1.
thermal states. Tensor network methods work best for spin-chains, i.e., in one spatial dimension. Here, the MPO approximation allows for efficient classical simulation including, e.g., the efficient approximation of MPO observables.

As a last remark we comment on the positivity of MPOs. In general, one cannot practically check whether or not an MPO is positive-semidefinite and, hence, can be a density operator [49]. However, for the thermal state MPO approximations one can easily circumvent this issue by first approximating $e^{-\beta H/2}$ and then squaring the MPO at the cost of squaring the bond dimension [33].

D. Phase transitions

Expectation values and thermodynamic potentials of thermal states of finite systems are differentiable with respect to the Hamiltonian couplings and do not have non-analyticities. In contrast, in nature, we observe abrupt changes and discontinuities of the thermodynamic potentials and their derivatives. The solution to this apparent contradiction relies in the fact that these discontinuities only appear in the limit of infinitely large system sizes, usually denoted as the thermodynamic limit. This is actually one of the reasons why it is so difficult to prove the existence of phase transitions.

Hence, showing some behaviour for the scaling of the covariance for any system size can help to discard the existence of phase transitions. This is the case of the clustering of correlations proven in Theorem 1. It discards the possibility of a phase transition above the critical temperature, i.e. where $\beta < \beta^*$ [12].

In this context, it is interesting to mention the existence of spontaneous magnetization at sufficiently low temperatures $\beta > \beta_{\text{FSS}}$ in a relevant family of spin systems in 3 or more spatial dimensions [23]. This family of models includes Hamiltonians as the XX model and the Heisenberg antiferromagnetic model with spin 1, 3/2, ... The threshold temperature $\beta_{\text{FSS}}$ has a non-trivial expression given in Ref. [23]. Note that the above statement simultaneously discards the existence of phase transitions at the very low temperature regime, $\beta < \beta_{\text{FSS}}$, for this type of models, and ensures the existence of a critical point below the disordered phase such that its Curie inverse temperature fulfills $\beta_{\text{FSS}} > \beta_c > \beta^*$.\[V. ENERGY DISTRIBUTION OF THERMAL STATES\]

Another important property of thermal states is their energy distribution. The mean energy of a thermal state is given by

$$U(T) := \text{Tr} \left( H g(T^{-1}) \right). \quad (21)$$

For or short ranged Hamiltonians this quantity scales as the volume $N = |\mathcal{V}|$. It is then common to use the energy density, which is defined as the energy per site,

$$u(T) := U(T)/N. \quad (22)$$

A first question is what the qualitative relation between energy and temperature is. The heat capacity and specific heat capacity of the system at temperature $T$ are the quantities that tell us how much energy is necessary to increase the temperature of the system by one unit and are defined as

$$C(T) := \frac{dU(T)}{dT} \bigg|_{T=T^*}, \quad c(T) := \frac{du(T)}{dT} \bigg|_{T=T^*}, \quad (23)$$

respectively. A straightforward calculation leads to the identity

$$C(T) = \frac{\Delta E(T)^2}{T^2} \geq 0, \quad (24)$$

where $\Delta E^2(T) = \text{Tr}[H^2 g(\beta)] - (\text{Tr}[H g(\beta)])^2$ is the variance of the energy. Two salient comments regarding Eq. (24) are in order. First, the positivity of the heat capacity shows that energy is a monotonically increasing function of temperature for any system, matching with our daily life intuition. This is in fact the reason why the energy-entropy diagrams presented in the book chapter [7] are convex, which is a crucial property to have a non-trivial theory of thermodynamics.

Second, we can see in Eq. (24) that the energy fluctuations of a thermal state do not scale with the energy of the system but with its square root. In other words, the energy distribution of thermal states becomes relatively thinner and thinner as the system size increases, and this happens irrespective of the Hamiltonian of the system. Note that this property is necessary in order for an equivalence of ensembles to be possible. This issue is discussed in Section VI.

It is interesting to point out that systems that are out of equilibrium and have a wide energy distribution cannot thermalize, that is, cannot equilibrate towards a Gibbs state. This is a consequence of the fact that the energy distribution of a system does not vary during the evolution and thermal states have relatively small energy fluctuations.

If we now focus on the relevant family of states that have a finite correlation length, it is even possible to show that the energy distribution converges to a Gaussian with increasing system size [21, 50].

Below, we state the latest result [21] applied to 2-local Hamiltonians, i.e., to Hamiltonians on cubic lattices. A cubic interaction graph has a vertex set $\mathcal{V} = [n]^D$ and two sites $v, w \in [n]^D$ are connected if $\sum_{i=1}^{D} |v_i - w_i| = 1$; see Figure 1 for $D = 2$.

Theorem 6 (Berry-Esseen bound [21, Lemma 8]). Let $H$ be a Hamiltonian (1) with cubic interaction graph $[n]^D$ with $N := n^D$ sites and $\rho$ a state with $(\xi, z)$-
exponentially decaying correlations (17). Moreover, let
\[ F(x) = \sum_{k: E_k \leq x} \langle k | \rho | k \rangle, \]  
(25)
\[ \mu = \text{Tr}(\rho H), \]  
(26)
\[ \sigma^2 = \text{Tr} \left( \rho (H - \mu)^2 \right) \]  
(27)
and define the Gaussian cumulative distribution function with mean \( \mu \) and variance \( \sigma^2 \) by
\[ G(x) = \frac{1}{\sqrt{2\pi \sigma^2}} \int_{-\infty}^{x} dy e^{-\frac{(y-x)^2}{2\sigma^2}}. \]  
(28)
Then
\[ \sup_x |F(x) - G(x)| \leq C \frac{\ln^2(N)}{\sqrt{N}}, \]  
(29)
where \( C \) is a constant that depends only on \( \xi, x \), and the local Hilbert-space dimension.

Hence, the distance between the cumulative distributions \( F \) and \( G \) can be made arbitrarily small in \( L_\infty \)-norm for sufficiently large system sizes \( N \). Note that the theorem all states with clustering of correlations, irrespective of being thermal.

The Gaussian distribution has an exponential decay outside an energy windows of a width scaling as \( \sigma \sim \sqrt{N} \). Hence, the theorem also suggests such a decay for states with \( (\xi,z) \)-exponentially decaying correlations. However, the error term in Eq. (29) scales like \( \tilde{O}(1/\sqrt{N}) \) and, hence, such a decay is not implied. However, a (sub)exponential decay can be guaranteed using a version of a non-commutative Chernoff-Hoeffding inequality [51–53].

Let us now insert in Eq. (25) the maximally mixed state \( \rho = 1/d \), with \( d \) being the dimension of the Hilbert space. Then, \( F(x) \) becomes
\[ F(x) = \frac{1}{d} \int_{-\infty}^{x} \sum_k \delta(E - E_k) \, dE \]  
(30)
which is nothing but the cumulative distribution of the density of states. As the maximally mixed state is a product state, a corollary of Theorem 6 is that short-ranged Hamiltonians have a density of states that tends to a Gaussian in the thermodynamic limit.

**VI. EQUIVALENCE OF ENSEMBLES**

The question of equivalence of ensembles (EoE) has a long tradition in statistical physics. Gibbs stated that, in the thermodynamic limit, an observable has the same average value in both the canonical and the microcanonical ensemble [54, Chapter 10]; see also Ref. [55] for a recent rigorous treatment of classical systems. The argument given by Gibbs is that the energy fluctuations of the canonical ensemble (relatively) vanish in the limit of infinitely large systems.

In classical systems, the microcanonical ensemble describes systems at equilibrium with a well defined energy \( E \). It assigns the same probability to all the configurations of the system (points in phase space) compatible with that energy.

In quantum theory, however, for systems with a discrete energy spectrum, the classical definition of microcanonical ensemble breaks down, since there often is, if any, only a single physical configuration for a given energy. Hence, in quantum systems the notion of microcanonical states needs to be slightly changed and the system is not considered to have a well defined energy but a uniform distribution within a narrow energy window of width \( 2\Delta \). More specifically, the microcanonical ensemble or microcanonical state \( \cap_{E,\Delta} \) of a quantum systems is defined as the completely mixed state within the energy subspace spanned by all the eigenvectors with energy \( |E_k - E| \leq \Delta \) (see Fig. 4).

Let us mention that the microcanonical ensemble is equivalent to the principle of equal a priori probabilities, which states that, once at equilibrium, the system is equally likely to be found in any of its accessible states. This assumption lies at the heart of statistical mechanics since it allows for the computation of equilibrium expectation values by performing averages on the phase space. However, there is no reason in the laws of mechanics (and quantum mechanics) to suggest that the system explores its set of accessible states uniformly. Therefore, the equal a priori probabilities principle has to be put in by hand.

One of the main insights from the field of quantum information theory to statistical mechanics is the substitution of the equal-a-priori-probabilities-postulate by the use of typicality arguments [56, 57]. This issue is discussed in detail in [1, Chapter 17].

An *equivalence of ensembles* statement says that a certain state is locally indistinguishable from a thermal state with the right temperature. Such statements are often shown for the microcanonical state \( \cap_{E,\Delta} \), see Refs. [21, 22, 58] investigations of quantum lattice sys-
Theorem 7 (EoE [21, Theorem 1, special case]). Let $g(1/T)$ be the thermal state of a Hamiltonian (1) with cubic interaction graph $|n|^D$ and with energy density $u(T)$ (22) and specific heat capacity $c(T)$ (23) with $(\xi, z)$-exponentially decaying correlations (17).

Let $\cap eN.\xi.\Delta N$ be the microcanonical state with mean energy density $e$ specified by

$$|e - u(T)| \leq \frac{\sqrt{c(T)T^2}}{\sqrt{N}}$$

and energy spread $\delta \sqrt{N}$ specified by

$$C_1 \frac{\ln(N)^{2D}}{\sqrt{N}} \leq \frac{\delta}{\sqrt{c(T)T^2}} \leq 1,$$

where $N := n^D$ denotes the volume and $C_1$ a constant. Then, for a linear system size scaling as $n \in \Omega(1^{D+1/\xi^2})$,

$$\|\tau_{x, \delta} - g(1/T)^{S_i}\|_1 \leq \epsilon$$

for any cube $S_i$ of edge length $l$.

All implicit constants and $C_1$ depend on the temperature $T$, the correlation decay $(\xi, z)$, and the spatial and Hilbert space dimension $D$ and $d$ (explicitly given in Ref. [21]).

This theorem tells us that for an energy window that needs to have a width scaling roughly as $\Delta = \delta \sqrt{N} \sim \sqrt{N}$ and matching median energy $E = eN \approx U(T)$ the microcanonical state is locally indistinguishable from the thermal state whenever the total system large enough.

The original statement [21, Theorem 1] is more general (but also more technical): (i) it also holds for $k$-local Hamiltonians ($k$-body interactions) and (ii) for systems that are not translation-invariant. In the case of (ii) the trace distance (33) needs to be replace with a trace distance averaged over all translates of the cube $S_i = [l]^D$. This means that the EoE statement holds in most regions of the non-translation invariant lattice.

The proof [21] of Theorem 7 is based on an information theoretic result for quantum many-body systems: If a state $\rho$ has $(\xi, z)$-exponentially decaying correlations and $\tau$ is another state such that the relative entropy $S(\tau|\rho)$ has a certain sub-volume scaling then $\tau_{x, \delta} \approx \rho_{x, \delta}$ on average over all cubes of edge length $l$. The approximation error depends on the explicit scaling of $S(\tau|\rho)$. Then a bound on $S(\|eN.\partial N|g(\beta))$ is proven. For this proof the Berry-Esseen bound Theorem 6 is derived.

VII. CONCLUSIONS AND OUTLOOK

In this chapter we have reviewed several properties of thermal states of spin lattice Hamiltonians. We have seen that, in a regime of high temperatures and for gapped Hamiltonians at zero temperature, equilibrium states exhibit an exponential cluster. This fast decay of the correlations can be exploited in several ways. It allows for locally assigning temperature to a subsystem even in the presence of interactions, as well as for approximating expectation values of local operators in infinite systems by means of finite ones. Furthermore, clustering of correlations in the high temperature regime discards the existence of phase transitions within that regime and implies that thermal states can be efficiently represented by means of matrix product operators. We have finally seen that states with a finite correlation length have a Gaussian energy distribution and, in the case that they are thermal, cannot be distinguished by local observables from the microcanonical ensemble, fleshing out in such a way the equivalence of ensembles.

Let us conclude the chapter by mentioning the problems that we consider relevant in the field and still remain open. One of the issues where progress seems to be very difficult is the extension of the well established theorems that logically connect area-law for the entanglement entropy, gapped Hamiltonian, and exponential clustering of correlations to a number of spatial dimensions higher than one. We also noticed a lack of results in the direction of understanding how much correlated thermal states of local Hamiltonians can be. More explicitly, how far concrete models are from saturating the area law for the mutual information. While there has been an important effort to contrive local Hamiltonians with highly entangled ground states, little is known for thermal states.

Completely new physics is expected to appear if one goes beyond the assumption of short ranged interactions. In this respect, a class of relevant models that both appears frequently in nature and can be easily engineered, e.g. in ion traps, are systems with long range interactions. For those, most of the questions discussed above are unexplored. As it already happened for the Lieb-Robinson bounds [59–61], some of the above properties, e.g. some type of clustering of correlations, could, at least in spirit, be reproduced. Indeed, for fermionic spin lattices an algebraic correlation decay can be shown for power-law interactions at non-zero temperature [62].

An interesting feature of systems with long range interactions is that they do not have a finite correlation length and thereby the results on equivalence of ensembles presented above cannot be applied. This opens fundamental questions in the field of equilibration of closed quantum systems, since it is not obvious that the canonical ensemble will be an appropriate description of the equilibrium state [63]. The challenge of the equivalence of ensembles for states with a power law decay of the correlations yields another relevant question in the field.

Other than extending EoE statements to long range interactions it is also important to extend them to larger classes of states. Often, states in quantum experiments arise from quenched dynamics and is a largely open and
challenging problem to characterize the thermalization behaviour. Part of the problem is the equivalence of the equilibrium state (given by an infinite time average [56]) and the thermal state. For non-critical systems such a statement can indeed be proven [64].

Thermal states have been introduced at the beginning of this book chapter as states that maximize the von Neumann entropy given the energy as conserved quantity. However, in many relevant situations, in particular for integrable models evolving completely isolated from their environments (closed system dynamics), it is well known that the thermal state is not a good description of the equilibrium state. These type of systems require to consider additional conserved quantities and their equilibrium state is given by the so called Generalized Gibbs Ensemble (GGE), which is the state maximizing the entropy given a set of conserved quantities. In the recent years, several studies on the laws of thermodynamics when GGE states are taken as heat baths have been realized (see the book chapter [65]). However, their intrinsic properties are in general completely unknown: scaling of the correlations, the shape of the energy distribution, or the locality of the Lagrange multipliers (e.g. temperature and chemical potential). Characterizing these properties constitutes an extensive research endeavor.

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