Lecture notes on quantum thermal states

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Abstract

These are some notes on quantum thermal states of many-body systems, prepared as support of the lectures in the "Quantum Thermodynamics Summer School" in Les Diablerets, Switzerland, 23-27th of August 2021.

I. INTRODUCTION

Here we will learn about some important properties of quantum many-body systems in thermal equilibrium. That is, we focus on

$$\rho_\beta = \frac{e^{-\beta H}}{Z}, \tag{1}$$

where H is the Hamiltonian, β is the inverse temperature and $Z \equiv \text{Tr}[e^{-\beta H}]$ is the partition function.

In previous lectures from this school, you may have studied properties of either small systems of few particles, or IID/non-interacting ensembles of many particles, such as $\rho_\beta = (\frac{e^{-\beta H}}{Z})^{\otimes N}$. We now start taking into account the interaction between the many particles. That is, we focus on a single Hamiltonian for the N particles, in which we restrict the interactions to be short-ranged or local.

A "local Hamiltonian" is a Hermitian operator H in the Hilbert space of N d-dimensional particles $(\mathbb{C}^d)^{\otimes N}$. It is defined as a sum of terms

$$H = \sum_i h_i \otimes \mathbb{I}, \tag{2}$$

each of which has bounded strength and support (i.e. acts non-trivially) on at most k particles. In what follows we will just write the terms as h_i for simplicity. These constitute the individual interactions, which are typically arranged in a lattice of a small dimension. A simple example is the transverse-field Ising model in one dimension with open BCs

$$H_{\text{Is}} = \sum_{j=1}^{N-1} \left(J\sigma_j^X \sigma_{j+1}^X + h\sigma_j^Z \right) + h\sigma_N^Z. \tag{3}$$

Here, $k = 2$ and the interactions are arranged on a 1D chain.

Of course this definition is very general, and involves many different models describing a wide range of situations. The only thing they have in common is the *locality* of the interactions. We thus aim to understand mathematically how does this fact alone universally constrain the physics. There are many different specific questions one could explore. In this note we describe two related ones, relevant for quantum thermodynamics:

- What are the correlations between the different parts of the thermal state? How are they distributed?

- What form do the subsystems of a thermal state take? How are they related to local Gibbs states? How can we approximate them?

A. Some motivation

Many of the most commonly studied quantum settings and current experimental platforms are described by some many-body local Hamiltonian. Their thermal states are particularly interesting for many reasons:

- It is one of the most **ubiquitous** states of quantum matter: typical experiments happen at finite temperature, where your quantum system is weakly coupled to some external radiation field that drives it to the thermal state.

- As we will also see, the thermal state is also important when studying not just systems with an external bath, but also in the evolution of **isolated** quantum systems, even in pure states: in generic cases, these end up being "their own bath", and the individual subsystems thermalize to the Gibbs ensemble.

- From a general condensed matter/material science standpoint, we are very interested in numerous questions about the physics at **finite temperature**: How are conserved quantities (e.g. charge, energy) propagated in a state close to equilibrium? How does the system respond to small or large perturbations away from equilibrium?

- Thermal states display interesting **phase transitions** in certain (low) temperature regimes (e.g. Ising model in 2D). It is thus interesting to study what are their universal properties both in and away from the critical points.

- Thermal states are also important for **computation**. For instance, being able to sample from the thermal distribution of local models is a typical subroutine for certain classical and quantum algorithms. Moreover, their low energy subspace is able to encode the solution to very hard computational problems (likely even hard for a quantum computer!), so it is interesting to study how does this "complexity" change with temperature.

- Perhaps more excitingly: We are in the dawn of the age of **synthetic quantum**

matter, where many complex quantum systems can be directly studied in experiments e.g. cold atoms or superconducting qubits.

II. MATHEMATICAL PRELIMINARIES

A. Operator norms

A basic but very important mathematical tool in this context are the Schatten p-norms for operators, as well as the different inequalities between them. These norms are maps from the space of operators to $\mathbb{R}$, as $M \rightarrow ||M||_p$, that obey the usual properties

- Homogeneous: If α is a scalar, $||\alpha M||_p = |\alpha| ||M||_p$
- Positive: $||M||_p \geq 0$
- Definite: $||M||_p = 0 \iff M = 0$.
- Triangle inequality: $||M + N||_p \leq ||M||_p + ||N||_p$.

For a given operator M with singular values $\{\lambda_l^M\}$ and $p \in [1, \infty]$, they are defined as

$$||M||_p \equiv \mathrm{Tr}[|M|^p]^{\frac{1}{p}} = \left(\sum_l (\lambda_l^M)^p \right)^{\frac{1}{p}}. \tag{4}$$

The more important ones are the operator norm $||M||_\infty = \max_l \lambda_l^M$, the Hilbert-Schmidt 2-norm $||M||_2 = \mathrm{Tr}[MM^\dagger]^{1/2}$ and the 1-norm or trace norm

$$||M||_1 = \max_{||N|| \leq 1} \mathrm{Tr}[MN]. \tag{5}$$

Thus $|\mathrm{Tr}[M]| \leq ||M||_1$, with equality for positive operators (for states $\mathrm{Tr}[\rho] = ||\rho||_1 = 1$).

Typically we measure the "strength" of an observable with the operator norm, and the closeness of two quantum states with the trace norm $||\rho - \sigma||_1$, since it is related with the probability of distinguishing them under measurements. The 2-norm, on the other hand, is often the easiest one to compute. Also note the very important Hölder's inequality

$$||MN||_p \leq ||M||_{q_1} ||N||_{q_2}, \tag{6}$$

which holds for $\frac{1}{p} = \frac{1}{q_1} + \frac{1}{q_2}$ (e.g. $p = q_1 = 1, q_2 = \infty$). A particularly useful corollary of this result is the Cauchy-Schwarz inequality (**Q**: Can you see how it follows from Eq. (6)?)

$$|\mathrm{Tr}[M^\dagger N]|^2 \leq \mathrm{Tr}[MM^\dagger]\mathrm{Tr}[NN^\dagger]. \tag{7}$$

B. Information-theoretic quantities

Let us also define the von Neumann entropy for a state ρ

$$S(\rho) = -\mathrm{Tr}[\rho \log(\rho)], \tag{8}$$

as well as the Umegaki relative entropy

$$D(\rho|\sigma) = \mathrm{Tr}[\rho(\log \rho - \log \sigma)], \tag{9}$$

which, as the trace norm, is a measure of distinguishability of quantum states. It obeys Pinsker's inequality $D(\rho|\sigma) \geq \frac{1}{2}||\rho - \sigma||_1^2$.

From these, we can also define the quantum mutual information, which, given a bipartite state ρ^{AB} with $\mathrm{Tr}_B[\rho^{AB}] = \rho^A, \mathrm{Tr}_A[\rho^{AB}] = \rho^B$, quantifies the correlations between A and B

$$I(A:B)_\rho = S(\rho_A) + S(\rho_B) - S(\rho_{AB} = D(\rho_{AB})|\rho_A \otimes \rho_B). \tag{10}$$

III. CORRELATIONS

One of the more important questions when studying many body systems is: how and how much are the different parts correlated? Intuitively, the stronger these correlations, and the longer their range, the more complex a state is. However, for thermal states, we can expect that the locality of the interactions will constraint the complexity. More specifically, it will cause the correlations to be "localized", meaning that particles are only correlated with their vicinity. For a first intuition, consider

$$e^{-\beta H} = \mathbb{I} - \beta \sum_i h_i + \frac{\beta^2}{2} \sum_{i,j} h_i h_j + ... \tag{11}$$

That is, at very high temperatures we approach the trivial uncorrelated state $\propto \mathbb{I}$ and the leading order term includes only k-local couplings, with only higher order terms coupling far away particles. We thus expect that the correlations between particles will be weaker $i)$ the higher the temperature and $ii)$ the larger their distance on the interaction graph. There are many reasons to study this, but a perhaps particularly important one is that the localization of correlations is related to the existence and efficiency of tensor network algorithms [1].

Below we describe (and even prove) some ways in which these correlations are constrained.

A. Correlations between neighbouring regions: Thermal area law

We now prove a well known statement: the area law for thermal states (see [2] for the original reference). Let us partition our interaction graph into two subsets of particles A, B, with a thermal state ρ_β^{AB}. The proof starts with the very simple thermodynamic observation that the free energy F of the thermal state is lower than that of any other state, and in particular

$$F(\rho_\beta^{AB}) \leq F(\rho_\beta^A \otimes \rho_\beta^B). \tag{12}$$

Writing out the free energy explicitly as $F(\rho) = \mathrm{Tr}[\rho H] - \beta^{-1} S(\rho)$ and rearranging yields

$$S(\rho_\beta^{AB}) - S(\rho_\beta^A \otimes \rho_\beta^B) \leq \beta \left(\mathrm{Tr}[H \rho_\beta^A \otimes \rho_\beta^B] - \mathrm{Tr}[H \rho_\beta^{AB}] \right). \tag{13}$$

Given that the entropy is additive $S(\rho \otimes \sigma) = S(\rho) + S(\sigma)$ notice that the LHS is exactly the mutual information $I(A:B)_{\rho_\beta^{AB}}$ from Eq. (10). Now, since our Hamiltonian is local, we can write it as

$$H = H_A + H_B + H_I, \tag{14}$$

where H_A, H_B have support on A, B respectively, and H_I is the interaction between them (with support on both). By definition, the expectation values of H_A and H_B coincide on both states $\mathrm{Tr}[(H_A + H_B)\rho_\beta^A \otimes \rho_\beta^B] = \mathrm{Tr}[(H_A + H_B)\rho_\beta^{AB}]$, so that

$$\beta \left(\mathrm{Tr}[H \rho_\beta^A \otimes \rho_\beta^B] - \mathrm{Tr}[H \rho_\beta^{AB}] \right) = \beta \left(\mathrm{Tr}[H_I \rho_\beta^A \otimes \rho_\beta^B] - \mathrm{Tr}[H_I \rho_\beta^{AB}] \right). \tag{15}$$

Now we can use a few of the operator inequalities from Section II A to obtain

$$\mathrm{Tr}[H_I \rho_\beta^A \otimes \rho_\beta^B] - \mathrm{Tr}[H_I \rho_\beta^{AB}] \leq ||H_I(\rho_\beta^A \otimes \rho_\beta^B - \rho_\beta^{AB})||_1 \tag{16}$$

$$\leq ||H_I|| \times ||\rho_\beta^A \otimes \rho_\beta^B - \rho_\beta^{AB}||_1 \tag{17}$$

$$\leq ||H_I|| \times (||\rho_\beta^A \otimes \rho_\beta^B||_1 + ||\rho_\beta^{AB}||_1) = 2||H_I|| \tag{18}$$

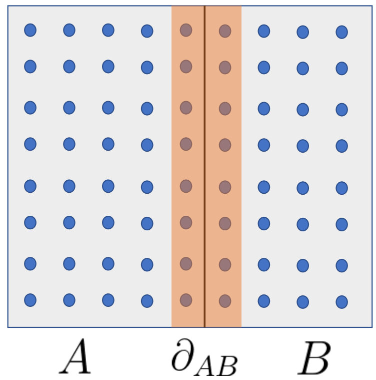
Putting all together we have the final result

$$I(A:B)_{\rho_\beta^{AB}} \leq 2\beta ||H_I||. \tag{19}$$

This is an *area law* for the mutual information of a thermal state: it says that the strength of the correlations of systems A, B does not depend on their size, but on their common boundary. For a local Hamiltonian, we have that

$$||H_I|| \leq 2k|\partial_{AB}| \times \max_i ||h_i||, \tag{20}$$

where $|\partial_{AB}|$ is the number of particles at the boundary of regions A, B, as defined by the interaction graph. Schematically:



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This is to be contrasted with the most general upper bound on the mutual information, which is $I(A:B) \leq \min\{\log(d_A), \log(d_B)\}$ (since $\log d_A \propto |A|$ this is a volume law instead).

What this suggests is that the correlations between A and B are localized around the mutual boundary, and that the bulks of A and B are mostly uncorrelated. That is, the only relevant information about A that B contains is about the region near the boundary.

Although this is by far the simplest, there are other versions of the thermal area law in the literature: with different temperature dependence [3] and for different measures of correlations [4, 5]. An important comment is that since they are upper bounds for all general models, they might not be tight in some cases. In fact, many physical models have a very different temperature dependence [6].

B. Long-range correlations: exponential decay

The fact that correlations between distant regions are very weak can be expressed in a different manner. Let C, D be regions such that their distance is $\text{dist}(C, D)$. We now look at the marginals on these regions $\text{Tr}_{\setminus(CD)}[\rho_\beta] = \rho_\beta^{CD}$ and its correlations. We expect that in general

$$I(C:D)_{\rho_\beta^{CD}} \leq f\left(\text{dist}(C, D)\right), \tag{21}$$

where f is some rapidly decaying function. In fact, in the following cases

- For any k-local interaction graph above a threshold temperature $\beta < \beta^*$, where β^* depends on parameters of the Hamiltonian (but not on its size) [3, 7].

- For 1D systems at all temperatures [8].

it can be shown that $f(l) \leq K|\partial_C||\partial_D|e^{-l/\xi}$, where $K > 0$ is some constant, $\partial_{C,D}$ is the size of the boundary and ξ is the thermal *correlation length* that depends on the temperature and other parameters, but not on l or system size. The proofs are relatively involved, so we refer the reader to the original references.

A more common but weaker condition is the decay of correlators (**Q:** can you see why this is weaker? Hint: use Pinsker's inequality and Eq. (10)). This usually takes the form

$$|\mathrm{Tr}[\rho_\beta M_C \otimes N_D] - \mathrm{Tr}[\rho_\beta M_C]\mathrm{Tr}[\rho_\beta N_D]| \leq K e^{-\mathrm{dist}(C,D)/\xi}, \tag{22}$$

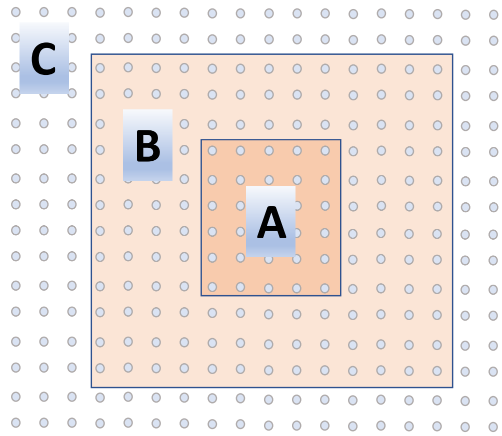
where here M_C and N_D have support on regions C, D, respectively.

This general property of correlation decay has been shown to be equivalent to the analiticity of the partition function [9]. Both in turn are related with the absence of phase thermal phase transitions (since it implies no long-range order): at them, the correlation function diverges and the partition function becomes non-analytic. There are known phase transitions at finite temperature (e.g. 2D Ising model), so the exponential decay does not hold for all thermal states at all temperatures.

This decay of correlations has as a wealth of physical consequences: it is associated with the phenomenon of equivalence of ensembles [10], with the validity of the central limit theorem and related results in thermal states [11], or even with some weak versions of the eigenstate thermalization hypothesis [12].

C. A refined correlation decay: Conditional mutual information

A significantly stronger known result about correlations in thermal states is the property of being an approximate *quantum Markov state* [13]. For this property, we need to consider three regions A, B, C such that B shields A from C, as



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We then define the conditional mutual information

$$I(A:C|B) = S(\rho_\beta^{AB}) + S(\rho_\beta^{BC}) - S(\rho_\beta^{ABC}) - S(\rho_\beta^{B}) \tag{23}$$

$$= I(A:BC)_{\rho_\beta} - I(A:B)_{\rho_\beta}. \tag{24}$$

This is a central quantity in quantum information theory, behind many non-trivial statements in quantum communication, cryptography and other fields (see Section 11.7 in [14] for more details). In a nutshell, it measures how much A and C share correlations that are *not* mediated by B. In other words: If this quantity is small, most of the correlations between A and C (which may be weak) are in reality correlations between A and B and B and C.

We thus expect that it becomes small as the size of B grows, and A, C are further apart. This is perhaps the strongest sense in which correlations can be localized, as for instance the decay of the mutual information follows by choosing $B = \varnothing$ to be the empty set.

The following two results are known

- In one dimension [15], $I(A:C|B) \leq c_1 |B| e^{-c_2\sqrt{|B|}}$
- In larger dimensions, and at high temperatures [16] $\beta \leq \beta^*$,

$$I(A:C|B) \leq k_1 \min\{|\partial A|, |\partial C|\} \left(\frac{\beta}{\beta^*}\right)^{-k_2 \times \mathrm{dist}(A,C)}$$

That is, it is known to decay (almost) exponentially in the distance between the two regions.

The significance of this, as well as the proofs involving it, are more technically involved and require some further quantum information tools (in particular, the idea of the Petz map [17]). Let us just briefly mention, however, that this is the only property that guarantees that the state on A, B, C can be reconstructed from ρ_{AB} by acting locally on B, such that $\mathcal{I}_A \otimes \mathcal{R}_{B\to BC}(\rho^{AB}) \simeq \rho^{ABC}$, with $\mathcal{R}_{B\to BC}$ some CP map taking only B as input.

IV. LOCALITY OF TEMPERATURE

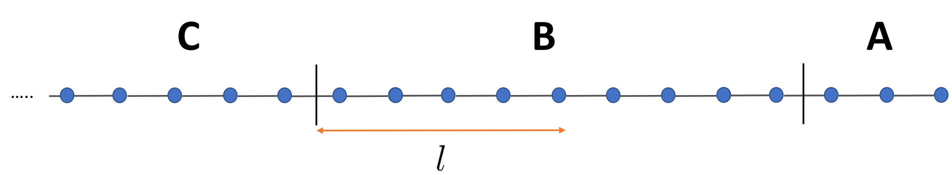
We have been looking at correlations between different parts. Now, we instead focus on what happens with individual subsystems. If the particles are non-interacting, it trivially holds that the marginal on A is the thermal state of H_A, $\mathrm{Tr}_{\setminus A}[\rho] = \frac{e^{-\beta H_A}}{Z_A}$ (we now drop the subscript β for simplicity of notation). The question is: how is this statement changed when we introduce local (and strong) interactions? Can we identify the state of a subsystem with some thermal state? How different is it from $\frac{e^{-\beta H_A}}{Z_A}$? This general question sometimes goes under the name of *locality of temperature* [7].

There are (to my knowledge) two complementary answers to this: the idea of *local indistinguishability* and also the notion of *Hamiltonian of mean force*. We will give a proof of the simplest instance of the first (in 1D), and briefly explain the second. Both statements seem to be relevant in the study of quantum thermodynamics of lattice models [18, 19].

A. A proof of local indistinguishability in one dimension

We now prove a statement about how to approximate the marginal of a thermal state on a small region, with a slightly larger region. It shares some steps and ideas that appear in other more fundamental questions including, for instance, the proof of the absence of phase transitions in 1D [9, 20] or of decay of correlations [8, 20]. We believe this makes it particularly suited for introductory notes like these.

Let us focus on the restricted setting of a chain, that we divide into three parts A, B, C, such that B is in the middle and A is a small subsystem at the end of the chain, as



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The Hamiltonian can be written as

$$H = H_A + H_{AB} + H_B + H_{BC} + H_C$$

. We have the full thermal state ρ, as well as a thermal state supported on A, B defined as

$$\rho_0^{AB} = \frac{e^{-\beta H_A + H_B + H_{AB}}}{Z_{AB}}, \tag{25}$$

that is, without the terms in H that have support in C (note that C may comprise most of the chain). One can also think of this as the marginal of the thermal state $\rho_0^{AB} \otimes \rho_0^C \equiv e^{-\beta(H_{AB}+H_C)}/Z_{AB}Z_C$ in which we have removed the interactions H_{BC} between AB and C.

Notice that $\rho_0^{AB} \neq \rho^{AB}$ due to the presence of H_{BC} (which is just a small local term). We now show that if B is large enough, these two states are indistinguishable on A: we aim for a small upper bound on

$$||\text{Tr}_{BC}[\rho] - \text{Tr}_B[\rho_0^{AB}]||_1 = \max_{||O_A|| \leq 1} |\text{Tr}[O_A(\rho - \rho_0^{AB} \otimes \rho_0^C)]|, \tag{26}$$

where O_A has support on A only, and the equality comes from the definition of the 1-norm. Now, let us define the following two operators

- $E_{BC} = e^{\beta H} e^{-\beta(H - H_{BC})}$,
- $E_{BC}^l = e^{\beta(H_C^l + H_B^l + H_{BC})} e^{-\beta(H_B^l + H_C^l)}$, where H_B^l and H_C^l are the terms of H_B and H_C that are a distance at least l from the boundary terms H_{BC}.

The second one E_{BC}^l is the same as E_{BC} but restricting the terms that appear in the exponents to be in the vicinity of H_{BC}. The parameter l is free and we can choose to our convenience.

A very important and fundamental result by Araki [20] (see also Appendix A of [15]) shows that there exists constants C_1, C_2 and q depending on β, J and $||H_{BC}||$ (but importantly, not on the size of any subsystem) such that

- $||E_{BC}|| \leq C_1$
- $||E_{BC} - E_{BC}^l|| \leq C_2 \frac{q^{1+l}}{(1+l)!}$

That is, the operator E_{BC} has bounded norm and, since we can approximate it by E_{BC}^l with e.g. some $l < \text{dist}(A, C)$, its support on region A is super-exponentially suppressed in l (due to the factorial, which always dominates over q^l). In what follows, we choose $l = |B|/2$. Notice that by definition $\rho_0^{AB} \otimes \rho_0^C = \frac{Z}{Z_{AB}Z_C} \rho E_{BC}$.

With the triangle inequality we can write

$$|\mathrm{Tr}[O_A(\rho - \rho_0^{AB} \otimes \rho_0^C)]| \le \left|\mathrm{Tr}[O_A(\rho - \frac{Z}{Z_{AB}Z_C}\rho E_{BC}^l)]\right| + \left|\mathrm{Tr}[O_A(\frac{Z}{Z_{AB}Z_C}\rho E_{BC}^l - \rho_0^{AB} \otimes \rho_0^C)]\right|. \tag{27}$$

Let us now upper-bound these two terms independently. The second can be bounded with Araki's result and Hölder's inequality applied twice.

$$\left|\mathrm{Tr}[O_A\frac{Z}{Z_{AB}Z_C}\rho E_{BC}^l - \rho_0^{AB} \otimes \rho_0^C)]\right| = \left|\mathrm{Tr}[O_A\frac{Z}{Z_{AB}Z_C}\rho(E_{BC}^l - E_{BC})]\right| \tag{28}$$

$$\le \frac{Z}{Z_{AB}Z_C}||O_A||||\rho||_1||E_{BC}^l - E_{BC}|| \tag{29}$$

$$\le \frac{Z}{Z_{AB}Z_C} \times C_2\frac{q^{1+l}}{(1+l)!}. \tag{30}$$

Since $\max\{\frac{Z}{Z_{AB}Z_C}, \frac{Z_{AB}Z_C}{Z}\} \le e^{\beta||H_{BC}||}$ (**Note:** showing this is part of the problem sets), which is a constant that only depends on β, k, J, we find that the second term is super-exponentially suppressed.

For the first term, we require the decay of correlations property from the previous section (which, as explained above, always holds in 1D). By Eq. (22) and since $l = |B|/2$,

$$\left|\mathrm{Tr}[O_A\rho E_{BC}^l] - \mathrm{Tr}[O_A\rho]\mathrm{Tr}[\rho E_{BC}^l]\right| \le Ke^{-\frac{|B|}{2\xi}}||E_{BC}^l|| \le 2KC_1e^{-\frac{|B|}{2\xi}}, \tag{31}$$

where for the last inequality we used $||E_{BC}^l|| \le ||E_{BC}|| + ||E_{BC}^l - E_{BC}|| \le 2C_1$, which holds for sufficiently large l. We can now write

$$\left|\mathrm{Tr}[O_A(\rho - \frac{Z}{Z_{AB}Z_C}\rho)E_{BC}^l]\right| \le \left|\mathrm{Tr}[O_A\rho] - \frac{Z}{Z_{AB}Z_C}\mathrm{Tr}[O_A\rho]\mathrm{Tr}[\rho E_{BC}^l]\right| + 2KC_1e^{-\frac{|B|}{2\xi}} \tag{32}$$

$$\le \left(1 - \frac{Z}{Z_{AB}Z_C}\mathrm{Tr}[\rho E_{BC}^l]\right) + 2KC_1e^{-\frac{|B|}{2\xi}}, \tag{33}$$

where we used the triangle inequality in the first line, and Hölder's inequality $\mathrm{Tr}[O_A\rho] \le ||O_A|| \le 1$ to get to the second. Finally, we can use Araki's result again after another application of (you guessed it!) Hölder's inequality

$$|\mathrm{Tr}[\rho E_{BC}^l] - \mathrm{Tr}[\rho E_{BC}]| \le ||E_{BC} - E_{BC}^l|| \le C_2\frac{q^{1+l}}{(1+l)!}, \tag{34}$$

and since $\mathrm{Tr}[\rho E_{BC}] = \frac{Z}{Z_{AB}Z_C} \le e^{\beta||H_{BC}||}$ we obtain

$$\left|\mathrm{Tr}[O_A(\rho - \frac{Z}{Z_{AB}Z_C}\rho E_{BC}^l)]\right| \le C_2e^{\beta||H_{BC}||}\frac{q^{1+l}}{(1+l)!} + 2KC_1e^{-\frac{|B|}{2\xi}}. \tag{35}$$

This finishes the proof. Putting everything together, we see that we have upper-bounded our target quantity in Eq. (26) by a small number related to the error term in the decay of correlations and Araki's result. Without worrying about the constants, and just on the leading exponential error, we can write the final result

$$||\mathrm{Tr}_{BC}[\rho] - \mathrm{Tr}_B[\rho_0^{AB}]||_1 \leq e^{-\Omega(|B|)}, \tag{36}$$

where $\Omega(x)$ is big-O notation for a function that grows at least as fast as x.

Here, for simplicity, we have only dealt with the simplest case of a 1D chain, where A is at the end of it. This proof, however, extends to more general situations [7, 21], provided that the decay of correlations property and some version of the Araki result hold (in fact, a different trick called quantum belief propagation [22] also suffices).

This means that the marginals of large thermal states do not depend much on what happens far away, and are very well approximated by the marginal of a much smaller thermal state (as long as $|B|$ is large enough). A straightforward consequence is that we do not need to know the whole state to compute local quantities. If we care about some kind of local order parameter, or want to compute heat flows between of some part and its surroundings, we can calculate this without having to diagonalize a huge matrix. This type of statement has implications for quantum algorithms for thermal states [21] and for tensor network representations [23]

B. Hamiltonian of mean force

We have seen that the marginal on A is close to the marginal of a smaller thermal state of the same Hamiltonian. However, can we also say that the marginal on A is the thermal state of some Hamiltonian on A only? This is obviously the case, since we can define

$$\tilde{H}_A \equiv \beta^{-1} \log \mathrm{Tr}_{\setminus A}[e^{-\beta H}]. \tag{37}$$

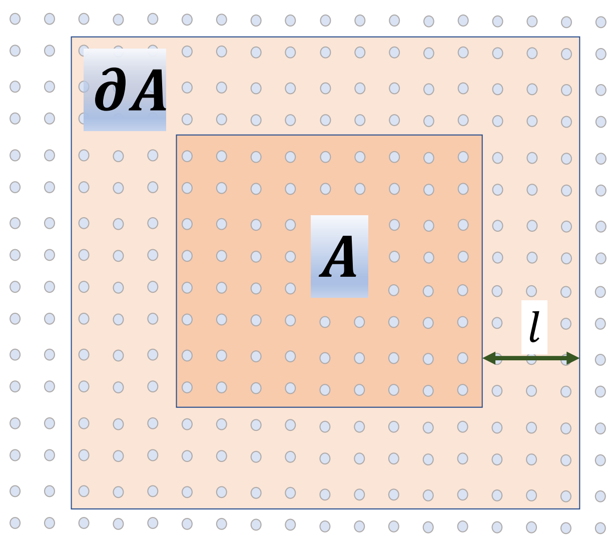
This is the so-called Hamiltonian of mean force [18]. The important question is: how does this compare to the "bare" Hamiltonian H_A, which disregards the interactions of A with the rest of the system? In other words, we would like to understand the operator $\Phi_A \equiv \tilde{H}_A - H_A$.

This turns out to be a difficult problem, which is related to the quantum Markov property and the decay of the conditional mutual information from Sec. III C. We now briefly describe a known result for high temperatures from [16], whose proof involves a very interesting (but also fairly involved) technique called the *linked cluster expansion*.

Since the interactions are local, it makes sense that, if the size of A is much larger than the interaction length k, most of the weight of Φ_A is localized around its boundary with the rest of the system, of size $|\partial A|$. A way to phrase this is: can we approximate Φ_A with another operator Φ_A^l that only has support on sites a distance l away from the boundary? Theorem 2 in [16] shows that, for any temperature β above a threshold one $\beta^* > 0$, one can define a Φ_A^l such that

$$||\Phi_A - \Phi_A^l|| \leq \frac{e}{4\beta} \frac{(\beta/\beta^*)^{l/k}}{1-\frac{\beta}{\beta^*}} |\partial A|. \tag{38}$$

That is, Φ_A can be exponentially well approximated with an operator localized around the boundary. This may be useful in analyzing quantities like heat and work in thermodynamic cycles within this strongly coupled regime. See below for an illustration: Φ_A^l will be supported in the light orange region only.



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V. FURTHER TECHNICAL TOOLS AND RESULTS

It appears at first that studying thermal states of general complex quantum models is a very challenging task in general. Hopefully here we have illustrated that this is not always the case, and that some non-trivial analytical statements can be made.

There is by now a fairly established list of techniques to study these problems, most of which deal with different simplifications of the matrix exponential of a local operator e^H

in different forms. We now provide a list of some of the more important ones that have appeared in the literature with a (very) rough description, with some of the references in which they appear.

- The result of Araki used above [20, 24], and higher dimensional extensions [25–29]. These deal with the norm and the locality of operators like $e^{-\beta H} e^{\beta(H+V)}$, as well as the "Euclidean time" Lieb-Robinson bound regarding operators such as $e^{-\beta H} V e^{\beta H}$.

- The Trotter decomposition, dealing with approximations of the form $e^{H_1+H_2} \sim e^{H_1} e^{H_2}$ [30, 31].

- The quantum belief propagation technique [15, 22] related to Araki's result. It shows that there is an operator Φ_V of bounded norm and quasilocal such that $e^{-\beta(H+V)} = \Phi_V e^{-\beta H} \Phi_V^\dagger$.

- The linked cluster expansion [7, 16, 32–34], which studies the individual terms of the Taylor expansion of $e^{-\beta H}$ as a sum of products of local terms (the "clusters"). It only converges above a threshold temperature β^*.

- Further polynomial approximations to the matrix exponential [3, 35].

Some of the most important of these only work well either in one dimension or at high temperatures. This is not a coincidence: we do not expect they will work at all temperatures, due to the presence of thermal phase transitions (such as the one of the classical 2D Ising model). It is an outstanding challenge to find alternative techniques to e.g. the cluster expansion that can be used in higher dimensions and low temperatures.

Let us conclude with some of the related questions in which recent progress has been made. Currently the study of many-body thermal states from a mathematical and information theoretic perspective is fairly active. Beyond those already mentioned, some interesting current topics are

- Classical simulation of thermal states [9], including tensor network approximations [3, 7, 23, 30, 36].

- Quantum simulation of thermal states [21, 37–40].

- Quantum algorithms for optimization problems, involving thermal sampling [41–43].

- Learning of quantum thermal states from local measurements [34, 44, 45].

This is list and the citations in it are very far from complete. Suggestions are very welcome!

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