Thermalization and Return to Equilibrium on Finite Quantum Lattice Systems

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Thermal states are the bedrock of statistical physics. Nevertheless, when and how they actually arise in closed quantum systems is not fully understood. We consider this question for systems with local Hamiltonians on finite quantum lattices. In a first step, we show that states with exponentially decaying correlations equilibrate after a quantum quench. Then, we show that the equilibrium state is locally equivalent to a thermal state, provided that the free energy of the equilibrium state is sufficiently small and the thermal state has exponentially decaying correlations. As an application, we look at a related important question: When are thermal states stable against noise? In other words, if we locally disturb a closed quantum system in a thermal state, will it return to thermal equilibrium? We rigorously show that this occurs when the correlations in the thermal state are exponentially decaying. All our results come with finite-size bounds, which are crucial for the growing field of quantum thermodynamics and other physical applications.

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To understand the strengths and limitations of statistical physics, it makes sense to derive it from physical principles, without *ad hoc* assumptions. Along these lines, over the past twenty years, ideas from quantum information have given new insights into the foundations of statistical physics [1–3]. In particular, some progress was made towards understanding how and when thermalization occurs [4–6]. A large class of states of systems with weak intensive interactions (e.g., one dimensional systems) were shown to thermalize [5]. In [6], thermalization was also proved for a large class of states, in the thermodynamic limit. (We will compare the results of [6] to our results in detail below.) More recently, the equivalence of the microcanonical and canonical ensemble (i.e., thermal state) was proved for finite quantum lattice systems, when correlations in the thermal state decay sufficiently quickly [7] (see, also, [6,8]).

Here, we prove thermalization results for closed quantum systems in two parts. First, we build upon previous equilibration results (e.g., Refs. [9,10]). A requirement for equilibration is that the effective dimension, defined below, is large. While there are physical arguments for this in some cases [11] (and it is true for most states drawn from the Haar measure on large subspaces [10]), there are no techniques for deciding whether a given initial state will equilibrate under a given Hamiltonian. Here, we prove that a large effective dimension is guaranteed for local Hamiltonian systems if the correlations in the initial state decay sufficiently quickly and the energy variance is sufficiently large. The latter is known for thermal states with intensive specific heat capacity and may, for large classes of states, be computed straightforwardly. The second part of thermalization is to show that the equilibrium state is locally indistinguishable from a thermal state. We prove that this occurs if the correlations in the corresponding thermal state decay sufficiently quickly and the relative entropy difference between the equilibrium state and the corresponding thermal state is sufficiently small.

As an application, we answer the following question. Given a closed quantum system that is initially in a thermal state, and supposing we locally quench or disturb it, will it reequilibrate to a thermal state? Understanding when thermal states are robust against local external noise is important, e.g., in decohering quantum simulations implemented in optical lattice systems (see, e.g., Ref. [12] and references therein), where noise can be caused by the absorption and reemission of a photon. Questions of reequilibration have a long tradition, and return to equilibrium was shown for infinite lattice systems in the seventies [13,14] by making transport assumptions: On an infinite lattice, information may leave a region and never return, which is not true for finite systems. This fundamental difference highlights the importance of finite-size considerations. We discuss the connection to results on infinite lattices further in [15].

Return to equilibrium was also shown for finite quantum systems coupled to infinite reservoirs after a coupling has been turned on [19,20], and a rough argument for stability of thermal states was given recently in terms of energy probability distributions in [21]. Here, we prove that a system in a thermal state, after being locally disturbed, reequilibrates to a thermal state provided correlations decay sufficiently quickly. In contrast to infinite lattice systems, our results give finite-size estimates and our methods and assumptions are entirely different. We emphasize that finite-size bounds are crucial for physical applications, particularly those in quantum thermodynamics [2], where thermal states are usually considered to be free resources. Understanding to what extent thermalization occurs will also affect protocols for extracting work using small quantum thermal machines.

Setting.—We consider a d-dimensional hypercubic lattice with $N = n^d$ sites. We suppose that each site has a d_{loc}-dimensional quantum system, e.g., a spin. We let H denote the (k-local) Hamiltonian; i.e., it has the form $H = \sum_i h_i$, where h_i acts only on lattice sites that are no more than k sites from i, i.e., only on sites j with $\mathrm{dist}(i, j) \leq k$. Further, we assume the h_i are bounded in operator norm and use units with $\|h_i\| \leq 1$ and $\hbar = k_B = 1$. We write $\rho(t) = e^{-iHt}\rho e^{iHt}$ for the state at time t and denote the time-average state by

$$\langle\rho\rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\rho(t). \tag{1}$$

We let σ^2 denote the energy variance of a state ρ with respect to a Hamiltonian H, $\sigma^2 = \mathrm{tr}[\rho H^2] - \mathrm{tr}^2[\rho H]$. We will be interested in subsystems, S, of the whole lattice and denote the rest by B—the bath or environment. We denote their Hilbert space dimensions by $d_S = d_{\mathrm{loc}}^{|S|}$ and $d_B = d_{\mathrm{loc}}^{|B|}$. Given a state of the whole system ρ, we write $\rho_S = \mathrm{tr}_B[\rho]$ and $\rho_B = \mathrm{tr}_S[\rho]$ for the reduced states of the subsystem and environment, respectively.

To discuss whether two states are close, we consider what one can measure in practice. Mostly, we will consider the local distinguishability of two states, ρ and τ, given by $\|\rho - \tau\|_S \coloneqq \|\rho_S - \tau_S\|_{\mathrm{tr}}$, where $\|\cdot\|_{\mathrm{tr}}$ is the trace distance. Our results extend naturally to coarse-grained observables, an example of which could be the magnetization of spins on a large region or even the whole lattice. We may write such an observable as $M = (1/m)\sum_{i=1}^m M_{S_i}$, where S_i are nonoverlapping subsystems and M_{S_i} acts only on subsystem S_i. For example, one could take the magnetization per spin $M = (1/N)\sum_i \sigma_z^i$. Then, local indistinguishability implies that expectation values of such observables are close: Assuming $\|M_{S_i}\| \leq C$, we have

$$|\mathrm{tr}[\rho M] - \mathrm{tr}[\sigma M]| \leq C \cdot \mathbb{E}_{S_i}\|\rho - \sigma\|_{S_i}, \tag{2}$$

where $\mathbb{E}_{S_i}$ denotes the average over subsystems S_i. Thus, we cover many physically realistic measurements.

Throughout, we will often consider states with exponentially decaying correlations. This is guaranteed, e.g., for thermal states above a critical temperature [22] and ground states of gapped k-local Hamiltonians [23]. We define exponentially decaying correlations as follows.

Definition 1.—A state ρ has exponentially decaying correlations if there is a correlation length $\xi > 0$ and a $K \geq 0$ (both independent of the system size N), such that, for any two lattice regions X and Y, one has

$$\max_{\substack{\mathrm{supp}[P]\subset X\\ \mathrm{supp}[Q]\subset Y\\ \|P\|,\|Q\|=1}} \left|\frac{\mathrm{tr}[\rho PQ] - \mathrm{tr}[\rho P]\mathrm{tr}[\rho Q]}{|X||Y|}\right| \leq K e^{-\mathrm{dist}(X,Y)/\xi}.$$

Here, the distance between the regions X and Y is $\mathrm{dist}(X, Y) = \min_{i\in X, j\in Y}\mathrm{dist}(i, j)$, where $\mathrm{dist}(\cdot,\cdot)$ is some metric on the lattice.

Equilibration.—Because of recurrences, a closed finite system will never truly equilibrate, not even locally. Hence, for finite systems, one asks a different question [10,11]: Does a system spend most of its time close to some fixed state? If we denote the fixed state by τ, this means that

$$D_S(\tau) \coloneqq \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\|\rho(t) - \tau\|_S \tag{3}$$

is small; i.e., for the majority of times, $\rho(t)$ and τ are locally indistinguishable. The most natural case is equilibration to the time-average state. For this case, it was proved that [10,24]

$$D_S(\langle\rho\rangle) \leq \frac{1}{2}\sqrt{\frac{D_G d_S^2}{d_{\mathrm{eff}}}}, \tag{4}$$

where d_S denotes the Hilbert space dimension of the subsystem S. Here, D_G is the degeneracy of the most degenerate energy gap [25], i.e., $D_G = 1$ if there are no degenerate energy gaps. Typically, one expects D_G to be small. Actually, the existence of degenerate energy gaps is a measure zero constraint on the Hamiltonian. Also in Eq. (4) is d_{eff}, known as the effective dimension, defined by

$$\frac{1}{d_{\mathrm{eff}}} = \sum_k \mathrm{tr}^2[P_k\rho], \tag{5}$$

where P_k is the energy projector corresponding to energy E_k. If the energies are nondegenerate, then $1/d_{\mathrm{eff}} = \mathrm{tr}[\langle\rho\rangle^2]$, i.e., the purity of the equilibrium state. Equation (4) implies that equilibration occurs when d_{eff} is large. The fraction of times when $\|\rho(t) - \langle\rho\rangle\|_S \geq \delta$ is at most $(d_S\sqrt{D_G})/(2\delta\sqrt{d_{\mathrm{eff}}})$, via Markov's inequality. Equation (4) is quite powerful: It holds for any decomposition of the total system into a subsystem S and bath B. This division need not correspond to a spatially localized subsystem. For example, one could consider multipoint correlation functions over arbitrary distances.

In Ref. [11], it was argued on physical grounds that we should expect d_{eff} to be exponentially large in the system size. The argument relied on the exponentially increasing density of energy levels for generic physical systems. Also, if the initial state is thermal, then $1/d_{\mathrm{eff}} \leq \mathrm{tr}[\rho(0)^2] \leq e^{\beta F}$, where $F = -1/\beta\ln(Z)$ is the free energy.

However, one cannot use these arguments in all physically interesting situations, for example, for a local (or global) quench. The free energy argument above is only useful for a highly mixed initial state, in contrast to initial pure or low temperature states, and there are simple examples where the initial state will not have an effective dimension that is exponentially large. For example, take the ground state of $H = -b\sum_i \sigma_x^i$. After quenching to $H = -J\sum_i \sigma_z^i \sigma_z^{i+1} - h\sum_i \sigma_z^i$, the effective dimension is, at most, $O(N^2)$ [26]. Furthermore, calculating the effective dimension means computing the overlaps of the state with energy eigenvectors, which is as hard as diagonalizing the Hamiltonian.

So we need concrete lower bounds on the effective dimension. Here, we prove such a bound.

Lemma 1.—Suppose the initial state ρ (or its time average $\langle\rho\rangle$) has exponentially decaying correlations as in Definition 1. Let the system evolve according to a bounded k-local Hamiltonian, and let ρ have energy variance σ^2 with respect to this Hamiltonian. Then, there is a constant C independent of N such that

$$\frac{1}{d_{\mathrm{eff}}} \le C\frac{\ln^{2d}(N)}{s^3\sqrt{N}}, \tag{6}$$

where $s = \sigma/\sqrt{N}$.

This is proved in [15] via a quantum Berry-Esseen theorem [7,27]. By assuming exponential decay of correlations, s is upper bounded independently of N. Often, it is also lower bounded, e.g., for thermal states with intensive specific heat capacity $c(\beta)$, which is given at inverse temperature β by $c(\beta) = \beta^2\sigma^2/N = \beta^2 s^2$. Furthermore, for many states (e.g., product states or matrix product states) it is straightforward to compute σ^2 so the question of equilibration may be answered directly, without knowing the overlap of the initial state with the energy eigenstates. That σ needs to be sufficiently large is reasonable: If the initial state is not sufficiently spread over many eigenstates, one cannot expect equilibration.

We may use Lemma 1 with Eq. (4) to show that equilibration occurs. One situation where this is interesting is a quench. If the initial state is a ground state of some Hamiltonian with exponentially decaying correlations (e.g., the ground state of a gapped k-local Hamiltonian), then after quenching to any other local Hamiltonian, equilibration will occur provided the energy variance σ^2 (with respect to the postquench Hamiltonian) is sufficiently large. Note that we need the total system to be quite large, with $\sqrt{N} \gg d_S^2$. Lemma 1 can also be applied to equilibration in the settings of [11,28].

An immediate application of Lemma 1 is to models studied in [29]. In the examples where weak thermalization and no thermalization are observed (see Figs. 1 and 2 in [29]), it is not clear whether equilibration will occur at all. However, in both cases, σ is $O(\sqrt{N})$, and we can apply Lemma 1 to lower bound the effective dimension. This guarantees that equilibration will occur for a finite model, provided there are not too many degenerate energy gaps, which is reasonable as the models are far from integrable.

Finally, we should mention that little is known about equilibration time scales. Rigorous bounds for general systems are extremely large [24,30,31] (these often involve d_{eff}, so our results apply). For some quadratic models, the time scale is much shorter [32,33]. Shorter time scales were also found for random Hamiltonians, states, or measurements [31,34–39]. Still, examples exist of reasonable translationally invariant models with extremely long equilibration time scales [40].

Thermalization.—In the previous section, we saw that equilibration occurs with great generality to the time-average state $\langle\rho\rangle$, but that is only part of thermalization. The second part is that the time-average state must be close to a thermal state. Thus, we need a practical way to decide whether, locally, $\langle\rho\rangle$ is close to a thermal state. The following Lemma (see [15] for a more quantitative version), recently obtained in Ref. [7], aids this by relating the local trace-norm distance of two states to their relative entropy difference.

Lemma 2.—Let σ be a state with exponentially decaying correlations as in Definition 1. Let $0 < \alpha < [1/(d+2)]$ and let $l \in \mathbb{N}$, $l^d \in o(n^{[(1-\alpha)/(d+1)]})$. Let τ be a state. If

$$S(\tau\|\sigma) \in o(N^{\{[1-(2+d)\alpha]/(d+1)\}}), \tag{7}$$

then there is a constant C, independent of N, such that the average local trace distance between σ and τ is bounded

$$\mathbb{E}_{S\in\mathcal{S}_l}\|\sigma - \tau\|_S \le \frac{C}{N^{\alpha/2}}, \tag{8}$$

where $\mathbb{E}_{S\in\mathcal{S}_l}$ denotes the average over all hypercubes on the lattice with length of side l.

Note that, even if the relative entropy difference between the two states increases with system size [as in Eq. (7)], the two states are locally close (on average, over all cubic subsystems of size l^d). Also, maybe surprisingly, the size of the subsystem need not be fixed but may increase as a power law in N. The bound in Eq. (8) tells us that (if N is sufficiently large), for the vast majority of subsystems $S \in \mathcal{S}_l$, the states σ_S and τ_S are close. For course-grained observables, as discussed below, one finds, e.g., for the magnetization per spin $M = (1/N)\sum_i \sigma_i^z$ (with $l = 1$),

$$|\mathrm{tr}[\sigma M] - \mathrm{tr}[\tau M]| \le \mathbb{E}_{S\in\mathcal{S}_l}\|\sigma - \tau\|_S, \tag{9}$$

so the bound in Eq. (8) directly gives a bound on the difference of expectation values in σ and τ. If both states are translationally invariant, the average is obsolete, and one has $\|\sigma - \tau\|_S \le CN^{-\alpha/2}$ for all cubic S of size l^d.

Let us move on to thermalization; i.e., we wish to show that $D_S(\rho_\beta)$ is small and, hence, that, for most times, $\rho(t)$ is locally close to the thermal state $\rho_\beta = \mathrm{e}^{-\beta H}/Z$, $Z = \mathrm{tr}[\mathrm{e}^{-\beta H}]$. We do this by combining Eq. (4) with Lemmas 1 and 2: Let the initial state ρ (or $\langle\rho\rangle$) have exponentially decaying correlations, evolve via a bounded k-local Hamiltonian H, and have energy variance σ^2. Fix $l \in \mathbb{N}$ and $\alpha \in \mathbb{R}$, $0 < \alpha < [1/(d+2)]$. Let the thermal state ρ_β have exponentially decaying correlations and suppose

$$S(\langle\rho\rangle\|\rho_\beta) \in o(N^{\{[1-(2+d)\alpha]/(d+1)\}}). \quad (10)$$

Then, there is a constant C independent of N such that (see [15] for details)

$$\mathbb{E}_{S\in\mathcal{S}_l} D_S(\rho_\beta) \le C\left(\sqrt{\frac{D_G}{s^3 N^{[d/(2d+4)]}}}+1\right)\frac{1}{N^{\alpha/2}}. \quad (11)$$

If ρ_β and $\langle\rho\rangle$ are translationally invariant, then $D_S(\rho_\beta)$ is upper bounded by the right-hand side for all $S \in \mathcal{S}_l$; i.e., thermalization occurs on every cubic subsystem of size l^d. This is true, e.g., when the Hamiltonian is translationally invariant with no degenerate energies. Without requiring translational invariance or making some other transport assumption, we cannot guarantee that every subsystem thermalizes. This is reasonable: We could consider models where a few small subsystems retain memory of their initial state.

In fact, we could replace the assumption that $\langle\rho\rangle$ be translationally invariant by assuming transport in the following sense. Suppose that, in terms of the time-average state, one cannot tell where a localized disturbance of the initial state had occurred. In other words, let Φ_i denote a local quantum channel on some region centred on i. Then, we demand that $\|\langle\Phi_i(\rho)\rangle - \langle\Phi_j(\rho)\rangle\|_S \le \epsilon \ll 1$ for any i, j and some small region S. Therefore, locally, the equilibrium state is indistinguishable from $\langle(1/N)\sum_i^N \Phi_i(\rho)\rangle$, which is translationally invariant. So the thermalization result Eq. (11) holds for the individual subsystem S with an extra ϵ on the right hand side. This follows from the triangle inequality. We discuss transport assumptions further in [15].

It is important to compare Eq. (11) to the results of [6], which proved that thermalization occurs in the thermodynamic limit, with a comparable condition on the time-average state. Here, we prove thermalization for the important case of finite systems, and we can give finite-size estimates. Furthermore, in [6], the thermal state must correspond to a unique phase. Instead, we assume that the thermal state has exponentially decaying correlations. This is always satisfied for $d = 1$ [41] and, for $d > 1$, if the temperature is above a critical temperature [22].

Finally, we note that the free energy of a state ρ at inverse temperature β is given by $F(\rho) = \mathrm{tr}[H\rho] - S(\rho)/\beta$, so $S(\langle\rho\rangle\|\rho_\beta) = \beta[F(\langle\rho\rangle) - F(\rho_\beta)]$. Thus, whenever the free energy of $\langle\rho\rangle$ is sufficiently small, $\langle\rho\rangle$ and ρ_β are locally close.

Stability of thermal states.—We can apply these results to some interesting examples. We will focus on the translationally invariant setting; i.e., we will assume that the time-average state $\langle\rho\rangle$ and the thermal state ρ_β are translationally invariant. This is true, e.g., when the Hamiltonian is translationally invariant and has no degenerate energies. As discussed above, translational invariance guarantees transport, without which we can not expect all subsystems to thermalize.

For the first example, suppose we have a system that was in a thermal state ρ_β, but was affected by a local process or some localized noise. We can model this by applying a local quantum channel [42]. Now, we see that the system locally returns to thermal equilibrium provided ρ_β had exponentially decaying correlations.

Theorem 3.—Let H be a bounded k-local Hamiltonian. Let ρ_β be a translationally invariant thermal state with exponentially decaying correlations as in Definition 1 and energy variance σ^2. Suppose Φ is a quantum channel acting nontrivially only on a cubic subsystem of fixed size. Fix $l \in \mathbb{N}$. Let $\rho = \Phi(\rho_\beta)$ evolve under H, and let $\langle\rho\rangle$ be translationally invariant. Then, the system locally rethermalizes: There is a constant C independent of N such that

$$D_S(\rho_\beta) \le C\left(\sqrt{\frac{D_G}{s^3 N^{[d/(2d+4)]}}}+1\right)\frac{1}{N^{[1/(2d+5)]}} \quad (12)$$

for all cubic subsystems S of size l^d; i.e., the system rethermalizes on any cubic subsystem of fixed size. In particular, this is true for the subsystem on which the channel Φ acted. See [15] for the proof.

As a second example, consider a system in thermal equilibrium. How much may the Hamiltonian change such that the system still equilibrates to a thermal state? The following theorem gives a rigorous answer.

Theorem 4.—Let H_0 be a Hamiltonian and $\rho = e^{-\beta H_0}/Z_0$ be the system's initial state, which we assume to have exponentially decaying correlations. Suppose that this state evolves under a bounded k-local Hamiltonian H and has energy variance σ^2 with respect to H. Let $\rho_\beta = \mathrm{e}^{-\beta H}/Z$, the thermal state corresponding to H, be translationally invariant and have exponentially decaying correlations. Let $\langle\rho\rangle$ be translationally invariant and $0 < \alpha < [1/(d+2)]$. If $\|H - H_0\| \in o(N^{\{[1-(2+d)\alpha]/(d+1)\}})$, then there is a constant C independent of N such that

$$D_S(\rho_\beta) \le C\left(\sqrt{\frac{D_G}{s^3 N^{[d/(2d+4)]}}}+1\right)\frac{1}{N^{\alpha/2}} \quad (13)$$

for all cubic subsystems S of size l^d. See [15] for a proof.

This implies that we can quench from Hamiltonian H_0 to Hamiltonian H, and we get local thermalization to ρ_β for any cubic subsystem of fixed size l^d provided the Hamiltonians are not too different. Maybe surprisingly, we are not restricted to local quenches: The difference between the Hamiltonians may grow as a power law in the system size N.

Discussion.—We have seen that, after locally perturbing a quantum system in a thermal state (with exponentially decaying correlations), the system equilibrates to a state indistinguishable from a thermal state on small subsystems of fixed size. This may not be true if there are long-range correlations in the initial state. Also, notice that one can easily construct counterexamples where an individual small subsystem will not return to thermal equilibrium after being perturbed without some form of transport assumption.

In [13], there are infinite lattice analogues of our findings (which are for finite systems). Infinite lattices are an entirely different setting because information can leave a subsystem and never return. Nevertheless, one may draw inspiration from [13] and try to generalize our work: For example, it may be possible to go beyond thermal states and show return to equilibrium of more general equilibrium states. We discuss how one may approach this problem further in [15].

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