Under what conditions do quantum systems thermalize? New insights from quantum information theory

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Quantum mechanics is generally regarded as a fundamental theory of physics. As such, it should be able to provide us with a microscopic explanation of all phenomena we observe in macroscopic systems, including irreversible processes such as thermalization. However, its unitary time evolution seems to be incompatible with irreversibility, leading to an apparent contradiction to many aspects of thermodynamics. This apparent contradiction is part of the long-standing problem of the emergence of classicality from quantum mechanics. The question of how quantum many-body systems in non-equilibrium eventually equilibrate and assume properties resembling the ones familiar from statistical mechanics has thus—quite unsurprisingly—a very long tradition [1].

Recently, this old question has received an enormous amount of attention [2–19], including our work [20–22], and there have been significant new insights. This renewed attention is partly driven by recent experimental advances, rendering it possible to probe coherent non-equilibrium dynamics under the controlled conditions offered by cold atoms in optical lattices [24], as well as by new mathematical and numerical techniques. Such systems can be seen as a first practically useful instance of a quantum simulator, in the sense that it simulates the dynamics under a meaningful well-defined local Hamiltonian and outperforms even the most elaborate, state-of-the art classical numerical techniques based on matrix-product states [24]. Clearly, rigorous analytic results are important to compare the experiments with theoretical predictions. Moreover, a good theoretical understanding of thermalization is the key to finding methods of preventing decoherence in such systems, an important step towards more fault-tolerant computation schemes.

A lot of the recent work on thermalization has been inspired by new mathematical tools from quantum information theory, like concentration of measure arguments [8–12, 16, 20, 21], quantum central limit theorems, and Lieb-Robinson bounds [4]. Their successful application to the fundamental questions of irreversibility is an impressive demonstration of the usefulness and broad applicability of ideas and methods from quantum information science. Our results [20–22] that we present are exactly in this line of thought:

Pure state quantum statistical mechanics. We consider a closed quantum system, consisting of a "system" S and a "bath" B evolving unitarily in time. That is, the global state of the full system is always a pure state that evolves reversibly. Thus, relaxation towards some equilibrium state in the usual sense is impossible, reflecting the apparent contradiction between quantum theory and thermodynamics mentioned above.

However, relaxation is still possible in a more general sense: we say that an observable equilibrates if its expectation value is close to some (equlibrium) value for almost all times and say that a subsystem S equilibrates if the expectation values of all local observables on this subsystem equilibrate. We are particularly interested in the case that S is a small subsystem of a larger quantum *many-body system*, but our results are not restricted to that situation.

A maximum entropy priciple from microscopic dynamics. As we have found in Ref. [22], applying very basic quantum information tools to this simple model can already yield surprising insights. Suppose we fix an arbitrary Hamiltonian $\mathscr{H}$ on the global system. Every Hamiltonian $\mathscr{H}$ defines a set of conserved observables. In the non-degenerate case, they are exactly the linear combinations of projectors onto the eigenstates of $\mathscr{H}$, in the degenerate case, they are the observables with support on the blocks corresponding to the degenerate subspaces. If the expectation value $\mathrm{Tr}[A\,\psi_t]$ of an observable A equilibrates in the sense defined above, then it must equilibrate towards its time average $\overline{\mathrm{Tr}[A\,\psi_t]} = \mathrm{Tr}[A\,\overline{\psi_t}]$.

Clearly, the time averaged state $\omega = \overline{\psi_t}$ of a state ψ_t undergoing unitary time evolution is given by $\omega = P(\psi_0)$, where $P(\psi_0) = \sum_j \pi_j \psi_0 \pi_j$, where the π_j are the projections onto (possibly degenerate) eigenspaces. Every state ρ that gives the same values for all conserved observables as ψ_0 satisfies $P(\psi_0) = P(\rho)$, and a simple application of the pinching inequality [22] on the Schur concave entropy function proves that $\omega = P(\psi_0)$ is the state having *maximal entropy* among all such states.

Theorem 1 (Maximum entropy principle [22])**.** *If the expectation value of an observable A equilibrates, then it necessarily equilibrates towards $\mathrm{Tr}[A\,\omega]$, where ω is the state that maximizes the von Neumann entropy, given the expectation values of all conserved quantities.*

While the mathematical content of the theorem is essentially obvious, it still proves an open conjecture from the physics literature [3, 18] that has attracted a considerable amount of attention.

Measure concentration and equilibration. Conventional statistical mechanics relies on ensemble averages; most no-

tably the microcanonical and canonical ensemble. In the quantum setting, the microcanonical ensemble is used in situations where all one knows about a closed physical system is that the value of some observable corresponding to a conserved quantity lies in some interval. The canonical ensemble applies to small subsystems of large microcanonical systems.

The phenomenon of measure concentration can be used to justify the microcanonical and canonical ensemble without added randomness, from nothing but pure Quantum Mechanics and the intrinsic quantum randomness due to entanglement with an environment. The results of Popescu at al. [10] suggest that the equal a priori probability postulate is dispensable: Instead of *assuming* that the microcanonical state yields a good description of the system it is possible to *prove* that for almost all pure states compatible with a microcanonical constraint of large systems all subsystems behave *as if the system were* in the corresponding microcanonical state. This is a statement about how *typical* individual instances of an ensemble are and was called *General Canonical Principle*.

In Ref. [20] we have extended the results of Ref. [10] to variances and higher moments, and in Refs. [20, 23] we have proved typicality for other ensembles, like the mean energy ensemble.

Moreover, under the assumption of non-degenerate energy gaps, Reimann and Linden et al. [9, 12] proved rigorously under which conditions equilibration (but not necessarily thermalization) happens. The important certificate quantifying the quality of equilibration is the *effective dimension* $d^{\mathrm{eff}}(\omega)$. It is a measure for how many energy eigenstates contribute significantly to the initial state. Whenever it is large, all small subsystems of a large quantum system equilibrate in trace norm. That is, the reduced state on the subsystem ρ_t^S remains within a small trace distance from a certain "equilibrium" state ω^S for almost all times. This means that the time average of their trace distance $\mathcal{D}(\psi_t^S, \omega^S)$ is small in the sense that [9]

$$\overline{\mathcal{D}(\psi_t^S, \omega^S)} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathrm{eff}}(\omega)}}, \tag{1}$$

where d_S is the dimension of the Hilbert space of the small system. A similar result for the speed of the reduced state

$$v^S(t) = \lim_{\delta t \to 0} \frac{\mathcal{D}(\rho_t^S, \rho_{t+\delta t}^S)}{\delta t} \tag{2}$$

was established by Linden et al. [8], namely

$$\overline{v^S(t)} \leq \| \mathscr{H}_S \otimes \mathbb{1} + \mathscr{H}_{SB} \|_\infty \sqrt{\frac{d_S^3}{d^{\mathrm{eff}}(\omega)}}. \tag{3}$$

Using concentration of measure techniques, it is possible to prove that in large quantum systems, almost all states have a large effective dimension $d^{\mathrm{eff}}(\omega)$ [9, 20], such that the right hand side of both (1) and (3) is typically small.

Absence of initial state independence. In systems that behave thermodynamically, the equilibrium expectation values of local observables on small subsystems should be independent of the initial state of the subsystem. In Ref. [22], we investigate under what conditions this is possible: we prove a sufficient condition for the *absence of initial state independence*.

Interestingly, a quantity R that we call *effective entanglement in the eigenbasis* plays a central role in our result. We show that whenever the effective entanglement in the eigenbasis is small, subsystem initial state independence cannot be satisfied. That is to say, small subsystems of large closed quantum systems remain distinguishable if they are initially well distinguishable even if the remainder (bath) of the system is started in precisely the same initial state.

More in detail, consider an initial product state $\psi_0 = \psi_0^S \otimes \psi_0^B$ on $S \otimes B$, and a global Hamiltonian $\mathscr{H}$ with eigenprojectors π_k. Our quantity is

$$R(\psi_0) := \sum_k \langle\psi_0|\pi_k|\psi_0\rangle \mathcal{D}\left(\frac{\mathrm{Tr}_B(\pi_k\psi_0\pi_k)}{\langle\psi_0|\pi_k|\psi_0\rangle}, \psi_0^S\right), \tag{4}$$

where $\mathcal{D}$ is the trace distance. If this is small, then all eigenprojectors π_k that have significant overlap with ψ_0 locally look very similar to ψ_0^S, which means that those relevant eigenstates contain very little entanglement. Our technical result is as follows: Suppose we have two global initial product states that are *different* on the subsystem S (on the bath, they may be the same, or be different, this does not matter). Then, if the quantity R of both initial states is small, and if the system equilibrates in both cases, *the corresponding equlibrium states on S are still distinguishable:*

Theorem 2 (Initial state dependence [22])**.** *The physical distinguishability of the two local time averaged states $\omega^{S(1)}$ and $\omega^{S(2)}$ of two pure initial product states*

$$\psi_0^{(i)} = \psi_0^{S(i)} \otimes \phi_0^{B(i)}, \quad i \in \{1, 2\}$$

evolving under a non-degenerate Hamiltonian $\mathscr{H}$ with low effective entanglement in the eigenbasis is large in the sense that

$$\mathcal{D}(\omega^{S(1)}, \omega^{S(2)}) \geq \mathcal{D}(\psi_0^{S(1)}, \psi_0^{S(2)}) - R(\psi_0^{(1)}) - R(\psi_0^{(2)}).$$

In Ref. [22], we also give an example of a natural many-body model that fulfills the premises of this theorem, even though it is *non-integrable* and hence expected to thermalize. That is to say, the model *locally equilibrates*, but the local equilibrium state *depends on the details of the initial state*. This is a surprising fact given the physical expectations for such models.

One may ask whether little entanglement in the energy eigenstates is *sufficient* to find initial states ψ_0 with small $R(\psi_0)$. In Ref. [22], we use concentration of measure arguments to answer this question in the positive: *Whenever the reduced energy eigenstates are all locally close to some basis, then there exist many initial states with small $R(\psi_0)$ and large $d^{\mathrm{eff}}(\omega)$.*

Equilibration and decoherence. In Ref. [21] we established a connection between the aforementioned results on equilibration with decoherence theory. In particular, we consider the physically relevant case of decoherence due to weak, but non-perturbative interaction with an environment (again treating system plus environment as a closed system).

The main result of Ref. [21] can be summarized as follows: Whenever $d^{\mathrm{eff}}(\omega)$ is large, coherent superpositions of eigenstates of the system Hamiltonian $\mathscr{H}_S$ with eigenvalue differences that are larger or comparable in size with the interaction energy cannot contribute significantly to the state of the subsystem for almost all times. That is, the corresponding off-diagonal elements of the reduced state ρ_t^S in the $\mathscr{H}_S$ eigenbasis must be small.

Theorem 3 (Decoherence under weak interaction [21])**.** *Consider a physical system evolving under a Hamiltonian of the form $\mathscr{H} = \mathscr{H}_S + \mathscr{H}_B + \mathscr{H}_{SB}$ and with non-degenerate energy gaps, where $\mathscr{H}_S$ and $\mathscr{H}_B$ act only on the system and bath respectively. All reduced states ρ^S satisfy*

$$\| \mathscr{H}_{SB} \|_\infty + v^S(t) \geq \max_{\{(k,l)\}} \sum_{(k,l)} |E_k^S - E_l^S| \, |\rho_{kl}^S| \tag{5}$$

$$\geq \max_{kl} |E_k^S - E_l^S| \, |\rho_{kl}^S|, \tag{6}$$

where ρ_{kl}^S are the matrix elements of the reduced state of the system in the $\mathscr{H}_S$ eigenbasis, and E_k^S are the corresponding eigenvalues of $\mathscr{H}_S$. The maximization in (5) *is performed over all decomposition of the index set $\{1, \ldots, d\}$ into a set of disjoint pairs $\{(k,l)\}$. (Note that it follows from* (3) *that $v^S(t)$ is small for almost all times.)*

The result is derived without making any assumptions about the structure of the bath or about the details of the interaction. It only uses the fact that the interaction is weak in a well-defined sense. The rigorous inequality that we established is stronger than naive perturbation theory, in the sense that it proves decoherence even if the interaction is much stronger than the gaps of the non-interaction Hamiltonian of the system plus bath $\mathscr{H}_S + \mathscr{H}_B$ and even if it is stronger (but not much stronger) than the gaps of $\mathscr{H}_S$. Moreover, our result remains meaningful even when the subsystem is large and its energy spectrum thus very dense. It then still implies that coherent superpositions of eigenstates with far apart energies (sometimes called Schödinger cat states) must decohere.

Conclusions. We have employed methods from quantum information theory to fundamental problems in quantum statistical mechanics. Our first result identifies a lack of entanglement in the energy eigenbasis as the reason for an "equilibration without thermalization" phenomenon: all local observables equilibrate but retain memory on their initial values for infinitely long time. As a second result, we have shown that quantum systems which interact weakly with the environment tend to evolve into convex combinations of energy eigenstates of their local Hamiltonian, thereby proving a generic decoherence mechanism from pure Schrödinger dynamics. Moreover, we have resolved an open problem from the physics literature by showing that the equilibrium state (resulting from unitary dynamics) must necessarily satisfy a maximum entropy principle.

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