# Observable Thermalization: Theory, Numerical and Analytical Evidence

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Predicting whether an observable will dynamically evolve to thermal equilibrium in an isolated quantum system is an important open problem, as it determines the applicability of thermodynamics and statistical mechanics. The Observable Thermalization framework has been proposed as a solution, characterizing observables that thermalize using an observable-specific maximum entropy principle. In this paper, we achieve three results. First, we confirm the dynamical relaxation of local observables towards maximum entropy, in a 1D Ising chain. Second, we provide the most general solution to the maximization problem and numerically verify some general predictions about equilibrium behavior in the same model. Third, we explore the emergence and physical meaning of an observable-specific notion of energy. Our results mark significant progress towards a fully predictive theory of thermalization in isolated quantum systems and open interesting questions about observable-specific thermodynamic quantities.



## I. INTRODUCTION

The concept of thermal equilibrium is at the heart of thermodynamics and statistical mechanics. Broadly speaking, if a system is at thermal equilibrium, we are rigorously justified to use thermodynamics and statistical physics to investigate its behavior. While this was originally intended to work at the macroscopic scale, i.e. for systems with an Avogadro number of degrees of freedom of $\mathcal{O}(10^{23})$, we now understand that both theories can work very well in regimes which are much closer to the microscopic scale — well below the Avogadro scale. Quantum Thermodynamics [1–4] is a direct example of this. Despite much progress, however, the necessary and sufficient conditions for the emergence of thermal equilibrium in quantum systems evolving unitarily are still not known. This long-standing problem has been open since the foundations of statistical mechanics were laid down at the end of the 19th century. Modern approaches to tackle the problem can be roughly organized in 4 major lines of inquiry: Quantum Chaos [5–8], Dynamical Equilibration [9–12], Typicality [13–16] and the Eigenstate Thermalization Hypothesis (ETH) [7, 17–20]. While each of them provides crucial inputs on *some* aspects of the thermalization problem, none of them is complete: they lack predictive power since they do not provide a complete characterization (necessary and sufficient) of the conditions for the dynamical emergence of thermal equilibrium.

The Observable Thermalization approach [21–23], which we investigate here, emerged as an attempt to address this issue. A full-fledged review of Observable Thermalization and how it relates to the other approaches is beyond the scope of the paper. For our purposes, it suffices to say that it stems from the attempt to incorporate the lessons from all the other lines of research to draw a coherent picture of thermalization and synthesize it into a framework that can be used to have new and testable predictions. In fact, Observable Thermalization has already allowed determining a large class of observables, called Hamiltonian Unbiased Observables (HUOs), which always exhibit thermal behavior, and for which the ETH can be analytically derived [21]. This was the first proof of the predictive power of this framework as it provides us with a consistent way of finding observables that always thermalize dynamically.

In this work, we test the Observable Thermalization approach and its predictive capabilities. First, we verify the dynamical emergence of the Maximum Observable Entropy principle, which states that the measurement statistics of an observable's eigenvalues, at equilibrium, is the one that maximizes its Shannon entropy under some constraints [21, 23]. We find good agreement with the envisioned behavior: the observable entropy exhibits a short transient followed by settling on a constrained maximum value, with small fluctuations around it. Second, by finding the generic solutions to the equilibrium equations of Observable Thermalization, we analytically extract a general prediction for the equilibrium behavior of thermalizing observables. We numerically confirm its validity for one-body observables, in a one-dimensional non-integrable transverse-field Ising model, and for a one-parameter family of initial states. In all cases considered, the agreement between data and predictions is extremely good. This is our second result. In turn, this leads to the emergence of a new quantity, whose physical role is studied and understood as an observable-specific notion of energy. This is our third result.

This constitutes significant progress towards a predictive theory for the emergence of thermal equilibrium in isolated quantum systems and it provides additional evidence in support of the Maximum Observable Entropy

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principle both as a dynamical mechanism and as a powerful predictive principle.

The paper is organized as follows. Sections II and III develop the theoretical and analytical arguments. In particular: section II provides a summary of the theory of Observable Thermalization, which also serves as a way to set language and notation; and, in section III we give the most general solution to the equilibrium equations, together with a new prediction of the theory, eq.(8). Section IV discusses the numerics and how the data supports the theory laid out before. Eventually, section V presents a general discussion about our results, and in section VI we draw some general conclusions.

## II. OBSERVABLE THERMAL EQUILIBRIUM

Within classical and quantum statistical mechanics, the notion of thermal equilibrium is deeply intertwined with Gibbs' ensemble: a system is at thermal equilibrium if and only if its equilibrium behavior is accurately described by statistical mechanics, via one of Gibbs' ensembles. As previously argued [21], this condition is experimentally inaccessible, unless we deal with very simple systems. One would have to probe a huge amount of observables, each with large statistics, to make a proper statement about the density matrix of the system under study. A more reasonable alternative is to recognize the predominant role of quantum measurements in extracting information from a quantum system. One then ascribes the condition of thermal equilibrium to the observed measurement statistics. This perspective, and its need, was argued for in ref.[21]. Here we provide additional support and strengthen the case for Observable Thermalization. We begin by introducing the relevant quantities and setting up notation.

### A. Notation

We have a quantum system described with a finite-dimensional Hilbert space $\mathcal{H}$ and we call $D = \dim\mathcal{H}$ its dimension. The system is made by $N$ repetitive units of interacting subsystems, each with Hilbert space $\mathcal{H}_1$ of dimension $d$. We thus have $\mathcal{H} = \otimes_{k=1}^{N}\mathcal{H}_1$ and $D = d^N$. The system is isolated and its evolution is generated by a time-independent Hamiltonian $H = \sum_{n=1}^{d^N} E_n \left|E_n\right\rangle\!\left\langle E_n\right|$, so that $\left|\psi_t\right\rangle = e^{-\frac{i}{\hbar}Ht}\left|\psi_0\right\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}\left|E_n\right\rangle$. Following von Neumann [16, 24] and subsequent authors [15, 19, 25–30], we also make the assumption that the fundamental frequencies $\omega_{nk} \coloneqq \frac{E_n - E_k}{\hbar}$ are unique. This is meant to exclude non-interacting Hamiltonians and it is not a particularly restrictive assumption, as it can be relaxed in several ways without affecting the core argument [27, 31]. Given some initial state $\left|\psi_0\right\rangle = \sum_n c_n \left|E_n\right\rangle$, it is well-known that an isolated quantum system can exhibit equilibration [10, 11, 32], in the following sense.

Consider an observable $A \coloneqq \sum_{j=1}^{n_A} a_j A_j$ where $A_j \coloneqq \sum_{s=1}^{d_j} \left|j,s\right\rangle\!\left\langle j,s\right|$, with $n_A$ the number of distinct eigenvalues, $d_j = \operatorname{Tr} A_j$ the number of degeneracies in the eigenspace corresponding to the $j$-th eigenvalue and $\{\left|j,s\right\rangle\}$ one of the eigenbases of $A$. Then, its eigenvalues' probability distribution is given by $\{p_j(t) \coloneqq \langle A_j\rangle(t) = \langle\psi_t|A_j|\psi_t\rangle\}_{j=1}^{n_A}$. We say that $p_j(t)$ has equilibrated when, after some characteristic equilibration time-scale $t > \tau_{eq}$, the time-dependent $p_j(t)$ will be close to $p_j^{DE} \coloneqq \langle A_j\rangle_{DE}$, the one computed on the diagonal ensemble $\rho_{DE} \coloneqq \overline{\left|\psi_t\right\rangle\!\left\langle\psi_t\right|}^{\infty} = \sum_n \left|c_n\right|^2 \left|E_n\right\rangle\!\left\langle E_n\right|$, where the overbar helps us define infinite-time averages $\overline{x_t}^T \coloneqq \frac{1}{T}\int_0^T x_t dt$ and $\overline{x_t}^{\infty} = \lim_{T\to\infty}\overline{x_t}^T$. Thus, to predict the equilibrium behavior of an isolated quantum system, $\rho_{DE}$ is our best bet. This, however, requires access to the energy eigenstates, and their occupation probabilities $|c_n|^2$. Something we know is practically unfeasible for many-body quantum systems, even for relatively low sizes.

### B. Observable Thermal Equilibrium

The quantum statistical mechanics of isolated systems rely on the microcanonical ensemble $\rho_{mc} \coloneqq \frac{1}{\mathcal{N}(E,\delta E)}\sum_{E_n\in I_{mc}} \left|E_n\right\rangle\!\left\langle E_n\right|$, where $I_{mc} \coloneqq \left[E - \frac{\delta E}{2}, E + \frac{\delta E}{2}\right]$, and $E$, $\delta E$ are, respectively, the average and standard deviation of the energy probability distribution. $\mathcal{N}(E,\delta E)$ is the number of energy eigenstates contained in $I_{mc}$. $\rho_{mc}$, however, can never be reached via unitary dynamics from any $\left|\psi_0\right\rangle$: $\{\left|E_n\right\rangle\!\left\langle E_n\right|\}_{n=1}^{d^N}$ is an exponentially large set of conserved quantities, which retains partial memory of the initial conditions. Thus, such thermal equilibrium is impossible for an isolated system, which evolves with a time-independent Hamiltonian. However, if we focus on sub-systems $\mathcal{H}_S = \otimes_{k=1}^{N_S}\mathcal{H}_1$, it is possible that $D_{Tr}\left(\rho_{DE}^S, \rho_{mc}^S\right) \ll 1$, where $D_{Tr}(\rho,\sigma)$ is the trace distance and $\rho^S$ is the reduced density matrix of the subsystem $S$. When this is the case, the statistics of *all observables* with support on $S$ can be extracted from $\rho_{mc}$, and we say that $S$ *is at thermal equilibrium.*

Using such a definition for thermal equilibrium as the basis of quantum statistical mechanics brings two practical issues. First, verifying its validity is exponentially hard in the size of the system. Hence, it is experimentally useless even for systems of modest sizes, say 50 qubits. Second, for such a condition to be proven wrong it is sufficient to have just one (only one) observable that departs from the predictions of statistical mechanics. In that case, even though its predictions might still hold for a large class of other observables, we simply cannot use it. In other words, we might not be using the ability to estimate various observables, because one of them cannot be predicted.

Observable Thermal Equilibrium is an alternative

thermal equilibrium definition that addresses both issues. By reflecting what happens in real experiments, it provides an observable-specific notion of thermal equilibrium which allows us to push the boundaries of statistical mechanics, and better understand its dynamical foundations. Defining the quantities

$$\epsilon_j^{DE}(t) \coloneqq \left|p_j(t) - p_j^{DE}\right|,$$
$$\epsilon_j^{mc} \coloneqq \left|p_j^{DE} - p_j^{mc}\right|,$$

we give the following, more practical, notion:

**Definition II.1** (Observable Thermal Equilibrium (OTE))**.** We say an observable $A$ is at thermal equilibrium when

$$\overline{\epsilon_j^{DE}(t)}^{\infty}, \epsilon_j^{mc} \leq \epsilon_A \ll 1 \quad \forall j \tag{1}$$

with $\epsilon_A > 0$ some small observable-specific quantity which is expected to be very small or vanish $\epsilon_A \to 0$ in the thermodynamic limit.

We emphasize that we are using a definition of equilibrium that addresses the whole probability distribution. This means that not only $\langle A \rangle$ will have a thermal behavior, but also all fluctuations like the standard deviation and all the higher moments $\langle A^n \rangle$.

### C. OTE vs Standard Thermal Equilibrium

If OTE is true for all observables with support on some subsystem $S$, then we return to the previous definition of thermal equilibrium for $\rho^S$. This is proven via the definition of trace distance: $D_{Tr}(\rho, \sigma) \coloneqq \max_O |\operatorname{Tr}(\rho O) - \operatorname{Tr}(\sigma O)|$. Indeed, since the max is taken over all observables, it also includes all projectors. Calling $\mathcal{A}_S$ the set of observables with support on $S$, if OTE is verified for all of them, we have $\epsilon_{\mathcal{A}_S} \coloneqq \max_{A \in \mathcal{A}_S} \epsilon_A \ll 1$. We thus conclude that, $D(\rho_{DE}^S, \rho_{mc}^S) \leq \epsilon_{\mathcal{A}_S} \ll 1$. OTE is, therefore, the core concept underlying the standard definition of thermal equilibrium. Indeed, it is quite easy to imagine situations in which the condition on the density matrix is violated because there is one observable that clearly violates OTE, while all the other ones still verify it. An example of a system in which this is true is the XXZ model, in the Many-Body Localized phase [33–35]. The local magnetization along $z$ never thermalizes, while the ones along $x$ and $y$ do. This was proven both analytically and numerically in ref.[23]. This example allows us to showcase the power of the Theory of Observable Thermalization and of the OTE. Indeed, quantum statistical mechanics breaks down in Many-Body Localized systems, so we cannot use it to study their equilibrium behavior. Observable Thermalization, however, allows us to use its prediction in the MBL phase, for some observables, namely those that satisfy OTE, thus pushing the boundary of statistical mechanics beyond its original domain of applicability.

### D. The three elements of the characterization problem

Looking at OTE from a mathematical perspective, the problem of finding the necessary and sufficient conditions for the emergence of OTE in an isolated quantum system is well posed if and only if the following three quantities are given: the initial state $|\psi_0\rangle$, the Hamiltonian $H$, and the observable $A$ (or, the set of projectors $\{A_j\}_{j=1}^{n_A}$). This can be easily proven, as follows. Given some $|\psi_0\rangle$ and some $H$, we can always find observables that do not satisfy the OTE ($[A, H] = 0$, such as the energy eigenprojectors) and observables that do satisfy the OTE (e.g., Hamiltonian Unbiased Observables, see ref.[21]) [36]. Given some $H$ and $A$, we can always find some $|\psi_0\rangle$ for which the OTE is true (e.g. thermally pure states, see ref.[37]), and some other ones for which the OTE condition is clearly false (superpositions of a few macroscopically different eigenenergies). Finally, given $A$ and $|\psi_0\rangle$, we can always find some $H$ which makes OTE true (e.g. $H$ such that $A$ is a HUO) and vice versa (when $[H, A] = 0$).

We conclude that OTE, and any other thermal equilibrium definition that builds on it, is a joint property of the triple $\mathbb{T} \coloneqq \{|\psi_0\rangle, A, H\}$, which we call *Thermal Equilibrium Characterization Triple*. Without specifying all three elements, the question is not well-defined and cannot be answered appropriately.

### E. Equilibrium Equations: A road to a predictive framework

Given a triple $\mathbb{T}$, when does $p_j(t)$ satisfy OTE? It is straightforward to see that, under experimentally realistic initial conditions [25, 38], the ETH is sufficient for OTE [19, 23]. Indeed, ETH's validity has been numerically checked in many cases [20, 39–44]. The necessity of the ETH has also been argued for [11, 45, 46], but it is currently less solid. While this clearly establishes the ETH as a core element of thermalization, this is a condition whose validity can be checked only through knowledge of the exact eigenstates. Hence, the problem of predicting which observables will satisfy OTE needs additional input.

Following Jaynes [47, 48], inference principles can help bridge the gap and constitute a principled, reliable, and established way to provide estimates in situations of lack of knowledge. In ref.[21], Anza and Vedral posited that one could characterize observables at equilibrium using the Maximum Observable Entropy principle. They then derive equilibrium equations to predict their distribution. Evidence of the validity of this theoretical framework, and its practical utility, were given in refs. [21, 22, 49]. Here we give a quick summary of the rationale behind the equilibrium equations, and how to derive them.

Given that our task is to estimate $p_j$, the Maximum Observable Entropy principle prescribes that our best bet is

$p_j^{eq}$, which is the probability distribution that maximizes the Shannon entropy $S_A \coloneqq -\sum_{j=1}^{n_A} p_j \log p_j$, compatibly with the validity of some set of constraints. How does one choose them? Given that the underlying dynamics is unitary, the memory of the initial conditions is written in the expectation value of the energy eigenstates $|c_n|^2$. These are constant quantities and one should therefore include all of them or any linear combination thereof. Such choice guarantees that we always get the exact answer [10, 11, 50], namely $p_j^{DE} \coloneqq \mathrm{Tr}(\rho_{DE} A_j)$. This, however, requires knowledge of the energy eigenstates. Moreover, due to the locality of physically reasonable observables, we do expect many of these constraints to not be relevant. A good approximation scheme is to trade the whole probability distribution $\{|c_n|^2\}$ with a suitable set of moments $\left\{\langle H^k\rangle = \sum_n |c_n|^2 E_n^k\right\}_{k=0}^{M}$. If $M = D-1$ this is equivalent to giving the full set $\left\{|c_n|^2\right\}_{n=0}^{D-1}$. For $M < D-1$ this provides a hierarchy of reasonable approximations, which was explicitly studied in ref. [50]. We now argue why, for experimentally realistic initial conditions, we believe $M = 1$ to be sufficient. As discussed in [25, 38], in the thermodynamic limit, we expect $|c_n|^2$ to be concentrated in an energy window which is small at the macroscopic scale (thermodynamic energy can be estimated with relatively low error), while still hosting a huge number of energy levels (the energy density is fantastically large). $|c_n|^2$ is therefore peaked around $\langle H\rangle$, and we expect its actual shape to be largely irrelevant. With such setup, the task is to find the distribution $p_j^{eq}$ which maximizes $S_A$ compatibly with the validity of the constraints fixing normalization and average energy. We reiterate that the standard notion of thermal equilibrium can be recovered from OTE by simply requiring the constrained maximization of the minimum among all possible observable entropies since $\min_A S_A = S_{\mathrm{vN}}$, where $S_{\mathrm{vN}} \coloneqq -\mathrm{Tr}(\rho \log \rho)$ is the von Neumann entropy. Hence, OTE is a generalization of the usual definition of thermal equilibrium.

The technical problem can be tackled using the Lagrange multipliers technique [51]. As discussed above, we keep only the normalization of probabilities and average energy constraints. After some algebraic manipulations, one obtains the following equilibrium equations, whose solution $p_j^{eq}$ is expected to characterize the equilibrium value of $p_j(t)$ when $t > \tau_{eq}$:

$$\mathrm{Tr}\left([A_j, H]\rho\right) \overset{\mathrm{eq}}{=} 0 \tag{2}$$

$$-p_j \log p_j \overset{\mathrm{eq}}{=} (1+\lambda_N)p_j + \lambda_E R_j \tag{3}$$

where $\lambda_E$ and $\lambda_N$ are, respectively, the Lagrange multipliers for the energy and normalization constraint, and

$$R_j \coloneqq \frac{1}{2}\mathrm{Tr}\left(\{A_j, H\}\rho\right). \tag{4}$$

Note that we do not expect these equations to be exactly satisfied for all times $t > \tau_{eq}$. However, we do expect them to hold, within some accuracy given by dynamical fluctuations, for most times. The first equation is about dynamical equilibration, i.e. it states the distribution must be invariant under the unitary dynamics generated by $H$. Indeed, using von Neumann's equation one has $i\hbar\frac{\partial}{\partial t}p_j = \mathrm{Tr}\left([A_j, H]\rho\right) \overset{\mathrm{eq}}{=} 0$. The second equation characterizes the shape of $p_j^{eq}$. For example, if we sum over the index $j$, we can see that the entropy of the equilibrium distribution has a thermodynamic flavor in the sense that it has a linear relation with the average energy:

$$S_A^{eq} = \log \mathcal{Z}_A + \beta_A E, \tag{5}$$

where $\beta_A \coloneqq \lambda_E$ plays the role of an observable-specific inverse temperature and, calling $\log \mathcal{Z}_A \coloneqq 1 + \lambda_N$, $\mathcal{Z}_A$ is an observable-specific partition function. All aspects of the derivation and a more detailed discussion on the equilibrium equations can be found in ref.[21].
Note furthermore that the object $R_j$ is an inner product between the operators $A_j$ and $H$ [52] and can also be expressed as

$$R_j = \mathrm{Cov}(A_j, H) + p_j E \tag{6}$$

by using the definition of the symmetrized covariance between two operators: $\mathrm{Cov}(X, Y) \coloneqq \langle X \circ Y\rangle - \langle X\rangle\langle Y\rangle$, where $X \circ Y \coloneqq \frac{XY+YX}{2}$ is the Jordan product between $X$ and $Y$.

We now discuss various strategies to solve the equilibrium equations, together with known analytical solutions.

## III. SOLVING THE EQUILIBRIUM EQUATIONS

Eqs.(2) and (3) are quite involved. Firstly, they both have parts that have an implicit dependence on $p_j$. Indeed, they depend explicitly on $\rho$, of which $p_j$ is simply a projection. Then, the second equation is highly nonlinear and implicit, containing $R_j$. Nevertheless, there is only one form of the equilibrium probability distribution which is compatible with the form of the Shannon entropy in eq.(5) above. This is the exponential family

$$p_j^{eq} = \begin{cases} \frac{1}{\mathcal{Z}_A} e^{-\lambda_E \varepsilon_j^{eq}} & \forall\, a_j \in \mathcal{I} \subseteq \sigma_A \\ 0 & \forall\, a_j \in \sigma_A / \mathcal{I} \end{cases} \tag{7}$$

where $\mathcal{Z}_A \coloneqq \sum_j e^{-\lambda_E \varepsilon_j^{eq}}$, $\varepsilon_j^{eq}$ is some energetic quantity such that $\sum_j p_j^{eq}\varepsilon_j^{eq} = E$, and $\mathcal{I}$ is an (improper) subset of the spectrum of $A$, $\sigma_A$. This follows straightforwardly from the Gibbs' inequality; see [53, 54]. Thus, if a solution exists it must have this form. However, $p_j^{eq}$ must also satisfy eq.(3); therefore, we plug the solution into this equation and obtain

$$R_j^{eq} = \varepsilon_j^{eq} p_j^{eq}. \tag{8}$$

This is a highly non-trivial prediction of the equilibrium equations and is required to hold for the solution to exist.

Thus, according to Observable Thermalization, at equilibrium, we must have $\langle A_j \circ H \rangle_{eq} = \varepsilon_j^{eq} p_j^{eq}$ for some $\varepsilon_j^{eq}$ yet to be characterized. To obtain a complete solution one still needs to fix the value of the Lagrange multiplier $\lambda_E$ by using the second constraint equation. That is, we need to find

$$\lambda_E \ : \ \sum_j p_j^{eq} \varepsilon_j^{eq} = -\frac{\partial \log \mathcal{Z}_A}{\partial \lambda_E} = E. \tag{9}$$

For a binary observable ($j \in \{0,1\}$) we can analytically solve this non-linear equation:

$$\lambda_E = \frac{1}{\delta\varepsilon} \operatorname{arctanh}\left(\frac{\bar{\varepsilon} - E}{\delta\varepsilon}\right) = \frac{1}{\varepsilon_1 - \varepsilon_0} \ln\left(\frac{\varepsilon_1 - E}{E - \varepsilon_0}\right), \tag{10}$$

where $\bar{\varepsilon} \coloneqq \frac{\varepsilon_1+\varepsilon_0}{2}$ and $\delta\varepsilon \coloneqq \frac{\varepsilon_1-\varepsilon_0}{2}$.
We now investigate the validity and consequences of eq.(8). In the next section, we will also provide numerical evidence supporting the arguments developed here.

### A. Hamiltonian Unbiased Observables

To understand eq.(8), we begin by looking at what happens when $\rho_{DE} \to |E_n\rangle\langle E_n|$, that is, we consider a microcanonical energy window with $\delta E \to 0$, such that in the limit it contains only one energy eigenstate. Physically, we do so because we believe the argument behind the ETH to be correct: thermalization occurs because thermal property can emerge already at the level of a single energy eigenstate. In this limiting case, we have that $R_j \to E_n p_j(E_n)$. This is indeed the form predicted by the equilibrium equations and, plugging it back into the second equilibrium equation we get $\varepsilon_j = E_n \ \forall j$ and therefore $p_j(E_n) = p_j^{eq} = \frac{1}{n_A}$. This happens when the observable $A$ is a Hamiltonian Unbiased Observable (HUO) [21], i.e., the observable energy eigenbases are mutually unbiased [55–58]. In this case, we have $R_j^{HUO} \overset{\text{eq}}{=} p_j^{HUO} E = \frac{E}{n_A}$, which implies $\mathrm{Cov}(A_j^{HUO}, H) \overset{\text{eq}}{=} 0$, by eq.(6). These were the solutions to the generic equilibrium equations originally found in [21, 23]. When initialized in out-of-equilibrium configurations, HUOs do exhibit fast equilibration and thermalization to the flat distribution, with truly maximal entropy $S_A = \log n_A$. HUOs are a very useful model to understand thermalization, for three reasons.

- First, the ETH holds for all of them, and this has been proven analytically in ref.[21].
- Second, in a statistically precise sense (Haar measure), most observables are expected to be quite close to being HUOs. This was proven in ref.[22], along with other statements clarifying the physical relevance of HUOs.
- Third, for Many-Body Localized systems, extensive sets of HUOs can be found analytically, and they are all quasi-local. This clearly shows the advantage of OTE against standard thermal equilibrium. Indeed, while it is true that MBL systems escape quantum statistical mechanics in the standard sense, there are several local observables that still exhibit OTE, even in the localized phase. They exhibit fast equilibration, and their long-time behavior is thermal. This was shown in ref.[23], and used in ref.[49].

### B. Beyond HUOs

While HUOs capture core aspects of observable thermalization, they have one major drawback: they are insensitive to the overall energy scale of the system. Technically, this is due to the fact that $R_j^{HUO}/p_j = E$, which does not depend on $j$. When this is plugged into the equilibrium equation, we see that the dependence of $p_j^{eq}$ on $j$ also disappears, thus leading to a flat distribution. We can also see this from eq.(6). HUOs are observables such that their projectors have no correlations with the Hamiltonian at equilibrium: $\mathrm{Cov}(A_j^{HUO}, H) \overset{\text{eq}}{=} 0$. We do not expect this to be true exactly for physical observables which, at equilibrium, do exhibit a smooth dependence on the energy scale of the system. Nevertheless, we believe the core mechanism to be approximately correct. In other words, while small, we expect a non-vanishing covariance between the observable projector $A_j$ and the Hamiltonian operator at equilibrium. The question thus becomes, is it possible to solve the equilibrium equations and use them to predict the equilibrium values of certain observables? Via eq.(8), this becomes a question about $R_j$, which we answer now.

Within a microcanonical energy window $I_{mc}$, $R_j \approx \sum_{E_n, E_m \in I_{mc}} c_n^* c_m \, e^{-i(E_m - E_n)t} \left(\frac{E_n+E_m}{2}\right) \langle E_n | A_j | E_m \rangle$ and $\left(\frac{E_n+E_m}{2}\right) \in I_{mc}$ so we found the following straightforward bound

$$\left(1 - \frac{\delta E}{2E}\right) p_j \lesssim \frac{R_j}{E} \lesssim \left(1 + \frac{\delta E}{2E}\right) p_j \tag{11}$$

This implies the existence of some $\tilde{\varepsilon}_j(t) \in I_{mc}$ such that $R_j(t) \approx \tilde{\varepsilon}_j(t) p_j(t)$. In the thermodynamic limit, we have $\delta E/E \ll 1$. So we expect the bound to be more and more stringent as we increase the size of our system. This means eq.(8) might indeed be reasonably true. We therefore define the ratio $\tilde{\varepsilon}_j(t) \coloneqq R_j(t)/p_j(t)$ which, in general, exists (unless $p_j(t) = 0$) and has the dimension of energy. While $\tilde{\epsilon}_j(t)$ exists, in principle it could fluctuate wildly, oscillate permanently, or exhibit other forms of dynamical behavior, rather than settling on a constant, as expected from eq.(8). We now provide numerical evidence that strongly supports $\tilde{\varepsilon}_j = \varepsilon_j$ and show that eq.(8) is indeed verified in the class of models we analyze.

This concludes the discussion about the general aspects of the theory and the generic solutions of the equilibrium

equations. We now present a numerical analysis that supports the theoretical picture. The physical interpretation of the quantity $\varepsilon_j$, together with a detailed discussion of the general solution found here, will be given later, in section V.

## IV. PREDICTIONS IN CONCRETE MODELS

The theory laid out in Sections II and III provides a set of principles to estimate the equilibrium probability distribution of observables. Here we test its predictions in a one-dimensional Ising model described by the Hamiltonian

$$H = \sum_{n=0}^{L-1} \left( J^z Z_n Z_{n+1} + B^z Z_n + B^x X_n \right), \qquad (12)$$

where $n$ is an index that runs over the $L$ lattice sites, and $Z_n \equiv \sigma_{z,n}$ etc., with $\sigma_{\alpha,n}$ ($\alpha = x, y, z$) representing the Pauli operator with Pauli matrix $\sigma_\alpha$ acting on the lattice site $n$, i.e.

$$\sigma_{\alpha,n} \coloneqq \mathbb{I}^{\otimes n} \otimes \sigma_\alpha \otimes \mathbb{I}^{\otimes (L-1-n)}. \qquad (13)$$

We use periodic boundary conditions, so that $\sigma_{\alpha,L} = \sigma_{\alpha,0}$. We choose the parameter values $(J^z, B^x, B^z) = (1, 0.9045, 0.8090)$, since they are guaranteed to give a robustly non-integrable model [42, 59]. We have considered system sizes up to $L = 10$ spins, and a class of initial states given by $|\psi_0(\theta_m)\rangle = R_y(\theta_m)^{\otimes L} |01\ldots01\rangle$, where $R_y(\theta) = \exp(-iY\theta/2)$ is the rotation operator along the $y$ axis [60] and $\theta_m = \frac{m-1}{19}\frac{\pi}{2}$. These states interpolate between the antiferromagnetic state along the $z$ direction ($\theta_1 = 0$) and the one along the $x$ direction ($\theta_{20} = \frac{\pi}{2}$). Note that the extremes are states of zero Shannon entropy for the observables $Z_n$ and $X_n$ respectively, thus maximally out of equilibrium for these observables. Throughout this study, we consider only local observables of the form given in eq.(13), whose coarse-grained eigen-projectors are

$$A_j^{\alpha,n} = \frac{\mathbb{I} + (-)^j \sigma_{\alpha,n}}{2} \quad (j = 0, 1). \qquad (14)$$

In the following, we present results only for the lattice site $n = 0$, as there is no difference between sites due to the translation invariance of the model.

We use exact diagonalization to obtain the state dynamics and then look at the behavior of the Shannon entropy of local observables $S_A(t) = -\sum_j p_j(t) \log p_j(t)$ with $p_j(t) = \langle\psi_t| A_j |\psi_t\rangle$. We observe that the entropy rapidly equilibrates to a stationary value $S_A^{\max}$, after an initial transient. This supports the use of a maximum entropy principle to determine the equilibrium probability distribution. Plots for observables $X_0$, $Y_0$ and $Z_0$ in a system with $L = 10$ spins and with initial state $|\psi(0)\rangle = |0101\ldots01\rangle$ are shown in fig.1. The antiferromagnetic state along $z$ is an eigenstate of $Z_0$, therefore this observable has zero Shannon entropy at $t = 0$. Its entropy quickly grows to the maximum and then settles on a stationary value. Instead, for $X_0$ and $Y_0$ the initial state chosen corresponds to maximal Shannon entropy $\log_2(2)$, and these observables equilibrate to a (slightly) lower value of entropy than their initial one. This is in agreement with the maximum entropy principle, as the presence of the constraints means $S_A = \log_2(2)$ is an out-of-equilibrium situation and the observables' entropy relaxes to the maximum value allowed $S_A^{max}$.

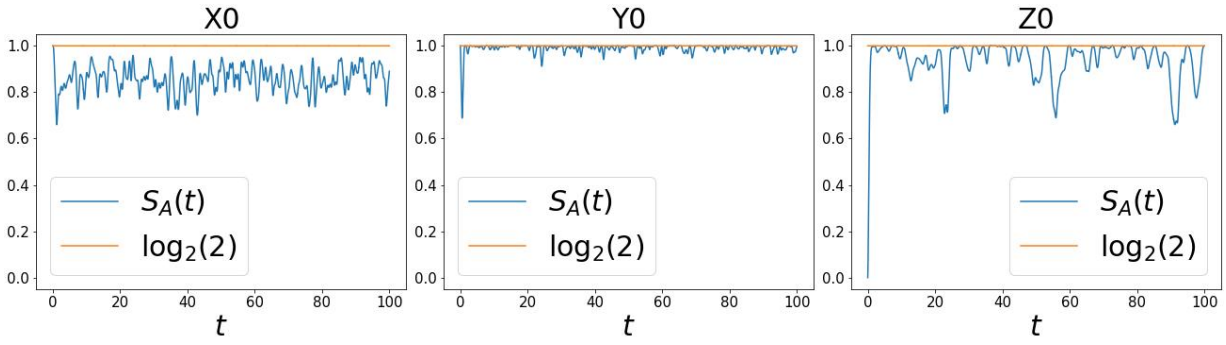
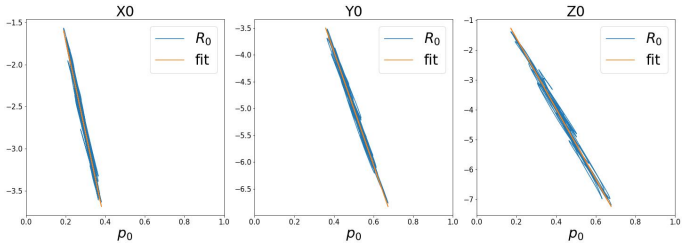



FIG. 1. Time evolution of the Shannon entropy of observables $X_0$, $Y_0$ and $Z_0$ for $L = 10$ and $|\psi(0)\rangle = |0101\ldots01\rangle$

We now look at the dynamical emergence of the prediction given by eq.(8). Since we expect $\varepsilon_j$ to be well defined at equilibrium, we look at its dynamic counterpart $\tilde{\varepsilon}_j(t) = R_j(t)/p_j(t)$. In principle, this can fluctuate wildly in out-of-equilibrium situations, due to the possibility of a vanishing denominator. However,

after some initial transient, we expect it to settle on a fixed value. To see if this is true, we look at the time-implicit plot $\{(x(t), y(t)) = (p_j(t), R_j(t))\}_t$. In fig.2 we show a few examples where eq.(8) is respected. We clearly see that points settle on a stable orbit described by the linear law $R_j(t) = \varepsilon_j p_j(t)$, within some degree of tolerance. We find this to hold for all observables and initial states analyzed here. This is a highly non-trivial prediction about the dynamical phenomenology of many-body quantum systems, which emerges directly from the equilibrium equations.

FIG. 2. Time-implicit plot of $R_0(t)$ against $p_0(t)$ for observables $X_0$, $Y_0$ and $Z_0$ for $L = 10$ and $|\psi(0)\rangle = |0101\ldots01\rangle$. Note that we are considering equilibrium quantities, as the transient has been removed from the data. Note also that the time-implicit plot for $(p_1(t), R_1(t))$ has the same behavior since $p_1 = 1 - p_0$ and $R_1 = E - R_0$.




Finally, since our goal is to predict the observables' probability distribution at equilibrium, we look at the time evolution of $p_j(t)$ and see that it equilibrates to its time average $\overline{p_j(t)}$ with small fluctuations around it. This means the first equilibrium equation, eq.(2) is satisfied, as the distribution is approximately constant under unitary evolution at equilibrium. We then extract $\varepsilon_j^{eq}$ from time-averages $\varepsilon_j^{eq} = \overline{R_j(t)}/\overline{p_j(t)}$, and the Lagrange multiplier $\lambda_E$ using eq.(10) (alternatively, one could also do a numerical optimization of the energy constraint equation, eq.(9)). Given these two quantities, we can now calculate $p^{eq} \propto e^{-\lambda_E \varepsilon_j}$ and compare it to the exact probability distribution after the transient is removed. The data shows excellent agreement with the theory, with $|\overline{p_j(t)} - p_j^{eq}| < 10^{-7}$, thus supporting the framework's validity. Fig.3 shows this for observables $X_0$, $Y_0$ and $Z_0$ in a system of size $L = 10$ and with initial state $|\psi(0)\rangle = |0101\ldots01\rangle$.

## V. DISCUSSION

We now discuss the results obtained in the previous section, with respect to the general theory outlined in section II and III.

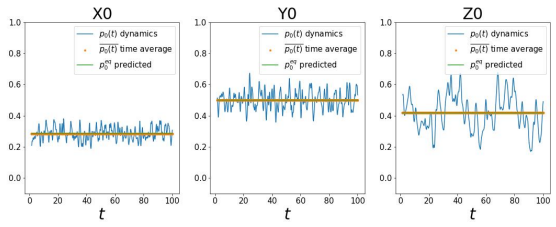



FIG. 3. Time evolution of the eigenvalue probability distribution $p_j$ of observables $X_0$, $Y_0$ and $Z_0$ for $L = 10$ and $|\psi(0)\rangle = |0101\ldots01\rangle$. Note that the transient has been removed from the data.

### A. Dynamical Emergence of MaxEnt

Observable Thermalization is founded on the principle of Maximum Observable Entropy. It essentially states that the equilibrium distribution we observe is the one given by a constrained maximum entropy principle, applied to the measurement statistics of the observable's eigenvalues $p_j$.

By looking at the full out-of-equilibrium dynamics of one-body observables for a one-parameter class of initial states, we observe a phenomenology compatible with the Maximum Observable Entropy principle: the entropy $S_A(t)$ rapidly relaxes to a stationary value, and then fluctuates around it. This constitutes good dynamical evidence that, at least for the model studied here, we can indeed use the Maximum Observable Entropy to predict the equilibrium value of one-body observables. This is our first result.

### B. Solution of the Equilibrium Equations and $R_j = \varepsilon_j^{eq} p_j$ prediction

Thanks to Gibbs' inequality, it is possible to give the most general solution to the Equilibrium Equations, eqs.(2) and (3), using the exponential family of probability distributions: $p_j^{eq} \propto e^{-\lambda_E \varepsilon_j}$. However, the quantities $\varepsilon_j$ are unknown and it is not clear what role they play. Using this, in section III we made a general prediction about equilibrium behavior: eq.8, namely $R_j = \varepsilon_j p_j$ for some constant $\varepsilon_j$. By studying time-implicit plots, see fig.2, we have observed that the prediction holds remarkably well. The points $(p_j(t), R_j(t))$ settle on an orbit described by a linear law. The value of $\varepsilon_j$ can then be extracted either by performing a linear fit or using time-averages, $\overline{R_j(t)}$ and $\overline{p_j(t)}$. Both give essentially the same value. The prediction is verified for all one-body observables and for the whole one-parameter family of initial states $|\psi_0(\theta_n)\rangle$. Confirming the validity of this prediction from Observable Thermalization is our second result.

While this gives us a dynamical interpretation of $\varepsilon_j$ as the proportionality constant between $R_j$ and $p_j$ at equilibrium, its physical meaning is yet to be understood. Thus, the question now becomes, what is $\varepsilon_j$ and what role

does it play? We address this in the next paragraph.

### C. The physical interpretation of $\varepsilon_j^{eq}$

In order to predict the equilibrium distribution $p_j^{eq}$, it is crucial to have knowledge of the object $\varepsilon_j^{eq}$, so we now provide a physical interpretation for it. In fact, this quantity has an important physical meaning at equilibrium: it is the (conditional) expected energy stored in $\mathcal{H}_j \subset \mathcal{H}$, the image of $A_j$. To see this we can compute the value of $\varepsilon_j$ given by the diagonal ensemble, $\varepsilon_j^{DE} = R_j^{DE}/p_j^{DE}$, since we expect $\varepsilon_j^{eq} \approx \varepsilon_j^{DE}$ (see section II):

$$\begin{aligned}\varepsilon_j^{DE} &:= \frac{R_j^{DE}}{p_j^{DE}} = \sum_n \frac{|c_n|^2 p_j(E_n)}{\sum_k |c_k|^2 p_j(E_k)} E_n \\ &=: \sum_n q_{n|j} E_n, \end{aligned} \tag{15}$$

with $R_j^{DE} := \frac{1}{2}\mathrm{Tr}\big(\{A_j, H\}\rho^{DE}\big)$ and $p_j(E_n) := \langle E_n| A_j |E_n\rangle$. We have also defined $q_{n|j} := \frac{|c_n|^2 p_j(E_n)}{\sum_k |c_k|^2 p_j(E_k)}$—the conditional probability of observing $E_n$, given the knowledge that, at equilibrium, our system inhabits the subspace $\mathcal{H}_j$. Indeed:

$$\begin{aligned}\mathrm{Prob}\left(E_n|a_j\right) :=& \frac{\mathrm{Prob}_{DE}(E_n)\mathrm{Prob}(a_j|E_n)}{\sum_k \mathrm{Prob}_{DE}(E_k)\mathrm{Prob}(a_j|E_k)} \qquad (16)\\ =& \frac{|c_n|^2 p_j(E_n)}{\sum_k |c_k|^2 p_j(E_k)} = q_{n|j} \qquad (17)\end{aligned}$$

Eventually, we can see $\varepsilon_j^{DE}$ is the expectation value of $E_n$ taken using $q_{n|j}$ as a probability distribution. We thus have that *$\varepsilon_j^{DE}$ is the conditional expected value of the energy, conditioned on the fact that the system inhabits the subspace $\mathcal{H}_j$*. In this statistical sense, $\varepsilon_j^{DE}$ is the amount of energy stored in the eigenspace $\mathcal{H}_j$ at fixed eigenvalue $a_j$. This physical interpretation relies on Bayes' theorem and, therefore, on the existence of a joint distribution $p_{DE}(E_n, a_j)$. Since in general $[H, A] \neq 0$, a unique joint distribution does not exist. Or, more accurately, the joint distribution depends on the order in which the measurements are performed: $p_{DE}(E_n, a_j) \neq p_{DE}(a_j, E_n)$. However, at equilibrium, $\langle [H, A]\rangle_{eq} = 0$, due to the first equilibrium equation eq.(2). So, while not generically correct, we expect our interpretation to hold, in a weak sense, at equilibrium. Moreover, while a unique joint distribution does not exist, once we've specified the order of the measurements, the joint distribution for the order "energy first, observable second" obviously exists. Thus, all manipulations required to interpret $q_{n|j}$ as a conditional probability distribution are allowed and follow from the existence of $p_{DE}(E_n, a_j)$. This is indeed confirmed by the fact that $q_{n|j}$ satisfies all the properties required by a conditional probability distribution $\mathrm{Prob}(E_n|a_j)$. These are $\sum_n \mathrm{Prob}(E_n|a_j) = 1$ and $\sum_j \mathrm{Prob}_{DE}(a_j)\mathbb{E}\left[E_n|a_j\right] = \langle H\rangle$. Here $\mathbb{E}[E_n|a_j] = \varepsilon_j^{DE}$ is the conditional expectation of the energy, given that we know the system to be in a state at given eigenvalue $a_j$. These are both satisfied by $q_{n|j}$:

$$\sum_n q_{n|j} = 1 \tag{18}$$

$$\sum_j p_j^{DE}\varepsilon_j^{DE} = \sum_j R_j^{DE} = E \tag{19}$$

Note that for HUOs $\varepsilon_j^{eq} = E\ \forall j$, which then turns $p_j^{eq}$ into a flat distribution. This goes well with the physical interpretation of $\varepsilon_j$ given above, and we can use it to understand why this happens, from a statistical mechanics perspective. Since $\sum_j p_j\varepsilon_j = E$, having a fixed $\varepsilon_j = E$ means that each subspace $\mathcal{H}_j$ hosts the same amount of average energy $\varepsilon_j = E$. The equilibrium distribution is flat because the various subspaces $\mathcal{H}_j$ are energetically equivalent and the dynamics of the system make no distinction between them. If, however, the conditional energies are not the same, the equilibrium distribution will be biased, favoring the ones with smaller conditional energy.

This is our third and most important result. Indeed, understanding $\varepsilon_j$ as a notion of energy for the observable under study paints a rather compelling picture for the emergence of statistical mechanics and thermodynamics.

To improve the predictivity of the theory, a necessary next step is to provide ways of computing $\varepsilon_j^{eq}$ from first principles rather than extracting it from the dynamics, for instance by using a perturbative approach. In fact, if an observable is HUO with respect to an unperturbed Hamiltonian whose eigenvalues and eigenvectors are known, it will be close to HUO when the perturbation is small and so one could use perturbation theory to compute its equilibrium probability distribution. Work is currently ongoing in this direction.

### D. Observable Thermodynamics

Eventually, we would like to discuss the inherently thermodynamic character of our equilibrium solutions, eq.(7). Since we obtain $S_A^{eq} = \log \mathcal{Z}_A + \beta E$, it is tempting to look at $\mathcal{Z}_A$ as an observable-specific partition function. Indeed, eq.9 have a distinctively thermodynamic flavor: it is the well-known relation among partition function, inverse temperature and internal energy. This suggests defining the *observable free energy* $F_A$ via $\mathcal{Z}_A =: e^{-\lambda_E F_A}$. We then have

$$F_A = E - T_A S_A\,, \tag{20}$$

where we have defined the observable temperature $T_A := \lambda_E^{-1}$, and re-introduced the index $A$ for clarity. This relation is essentially a form of energy conservation in the isolated system which, at equilibrium, turns into a relation between the observable entropy $S_A$, the observable

free energy $F_A$, and the average energy $E$. While the dynamic emergence of this relation is highly non-trivial, observing equilibration to the predictions of Observable Thermalization guarantees it. Again, this strengthens the case for observable-specific thermodynamics and statistical mechanics. However, in order to have a complete picture we would need a kinetic, or operational, interpretation of the observable-specific thermodynamic quantities $T_A$ and $F_A$. This is currently being developed and will be reported in future work.

## VI. CONCLUSIONS

Over 100 years after the foundation of statistical mechanics and thermodynamics we still do not know what are the necessary and sufficient conditions which guarantee the dynamical emergence of thermal equilibrium.
The theory of Observable Thermalization provides a predictive framework, based on the Maximum Observable Entropy principle, to tackle this issue. In this paper, we have investigated this theory's assumptions and predictions in a $1D$ model of spin 1/2. After giving the most general form of the solution of the equilibrium equations, we numerically confirmed the dynamical emergence of the Maximum Observable Entropy principle and confirmed the validity of a general prediction of the equilibrium equations, namely eq.(8). This is found to be true in all cases considered. The prediction led us to the remarkable emergence of the quantity $\varepsilon_j = R_j/p_j$. We have understood its physical meaning and its role in dynamical thermalization. $\varepsilon_j$ is the average amount of energy contained in $\mathcal{H}_j$, the subspace at fixed eigenvalue $a_j$. Therefore, it plays the role of energy for the observable under study, $A$. Once the $\varepsilon_j$ are correctly evaluated, the equilibrium distribution can be found by solving the optimization problem over the Lagrange multiplies $\lambda_E$, which establishes compatibility with the constraint of fixed average energy. Predictions arising from this method give remarkably good results for the equilibrium distribution, in all cases studied.

While we have made significant progress towards a fully predictive theory of thermalization, several avenues for future work remain open. We now mention a few of them. First, confirming the validity of the theoretical framework in other Hamiltonian models and for other observables would certainly bring additional support, and strengthen the case for the maximum observable entropy principle. Second, finding a generic way to compute the $\varepsilon_j$ from first principles, rather than from dynamics, is the most important step to achieve full predictive power. Third, the operational and kinetic interpretations of observable-specific thermodynamic quantities such as $T_A$ is certainly of interest. It would broaden our understanding of thermodynamics and expand the domain of applicability of statistical mechanics.

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