

# Thermal Equilibrium of a Macroscopic Quantum System in a Pure State

Sheldon Goldstein\*, David A. Huse<sup>†</sup>,  
Joel L. Lebowitz<sup>‡</sup> and Roderich Tumulka<sup>§</sup>

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## Abstract

We consider the notion of thermal equilibrium for an *individual* closed macroscopic quantum system in a pure state, i.e., described by a wave function. The macroscopic properties in thermal equilibrium of such a system, determined by its wave function, must be the same as those obtained from thermodynamics, e.g., spatial uniformity of temperature and chemical potential. When this is true we say that the system is in *macroscopic thermal equilibrium* (MATE). Such a system may however not be in *microscopic thermal equilibrium* (MITE). The latter requires that the reduced density matrices of small subsystems be close to those obtained from the microcanonical, equivalently the canonical, ensemble for the *whole* system. The distinction between MITE and MATE is particularly relevant for systems with many-body localization (MBL) for which the energy eigenfunctions fail to be in MITE while necessarily most of them, but not all, are in MATE. We note however that for generic macroscopic systems, including those with MBL, most wave functions in an energy shell are in both MATE and MITE. For a classical macroscopic system, MATE holds for most phase points on the energy surface, but MITE fails to hold for any phase point.

Key words: many-body localization, quantum statistical mechanics, canonical typicality, thermal equilibrium subspace, macro-observables, thermalization.

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\*Department of Mathematics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA. E-mail: oldstein@math.rutgers.edu

<sup>†</sup>Department of Physics, Princeton University, Jadwin Hall, Washington Road, Princeton, NJ 08544-0708, USA. E-mail: huse@princeton.edu

<sup>‡</sup>Departments of Mathematics and Physics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA. E-mail: lebowitz@math.rutgers.edu

<sup>§</sup>Department of Mathematics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA. E-mail: tumulka@math.rutgers.edu

# 1 Introduction

Thermal behavior of closed macroscopic systems in pure states has been widely studied in recent years; see e.g., [7, 28, 15, 41, 29, 30, 33, 21, 14, 31, 34, 32, 8], after some pioneering work even earlier [36, 45, 37, 6, 38, 42]. In particular, the importance of the *eigenstate thermalization hypothesis* (ETH) [6, 38] has become widely appreciated, see e.g., [33, 30, 21, 14, 16, 23, 32, 8]. It asserts, in one version, that all energy eigenstates (in a suitable energy shell) are thermal, i.e., assigning probability distributions to observables that are characteristic of thermal equilibrium. The ETH holds for many (but not all) macroscopic quantum systems. When it holds then the system, starting out of equilibrium, will thermalize (at least in the time average; see Section 4 below). Thus if a system does not thermalize it must have energy eigenfunctions that fail to be thermal.

An important case of this is that of many-body localization (MBL) [1, 3, 24], for which the Hamiltonian has (at least some) eigenfunctions that are in some way localized, so that, for any wave function, the component from these eigenfunctions will not spread but stay localized forever. For systems with MBL it has been argued that most (if not all) energy eigenfunctions (in suitable energy intervals) fail to be thermal, and there are in fact models for which this can be analytically [18], numerically [26], or perturbatively [2, 3, 35] seen to be the case. At the same time it has been argued [14] that most energy eigenstates must rather generally be thermal, in particular even for systems with MBL.

To reconcile these statements, we note that there are basically two notions of thermal equilibrium: a macroscopic notion of thermal equilibrium that we call MATE, and a more refined microscopic one that we call MITE. While most, but definitely not all, energy eigenstates of a system with MBL are in MATE (see Section 4), none, or nearly none, are in MITE [2, 3, 26, 18]. Nonetheless, most pure states in the energy shell are in both MATE and MITE, even for systems with MBL (see Sections 2 and 3). We say “most” for “all but a few” or “all except a set of small measure” (i.e., “an overwhelming majority of”); measures are taken to be normalized; the small measure, in fact, tends to 0 in the thermodynamic limit.

To be more precise, consider a finite, macroscopic, closed quantum system with Hilbert space  $\mathcal{H}$ . Let  $\mathcal{H}_{\text{mc}}$  be a micro-canonical energy shell, i.e., the subspace of  $\mathcal{H}$  spanned by the energy eigenstates with eigenvalues in an energy interval that is small on the macroscopic scale but contains many eigenvalues. The micro-canonical density matrix  $\hat{\rho}^{\text{mc}}$  is defined by  $\hat{\rho}^{\text{mc}} = (\dim \mathcal{H}_{\text{mc}})^{-1} \hat{P}_{\text{mc}}$  with  $\hat{P}_{\text{mc}}$  the projection to  $\mathcal{H}_{\text{mc}}$ . As usual, pure states in  $\mathcal{H}_{\text{mc}}$  are superpositions of energy eigenstates in  $\mathcal{H}_{\text{mc}}$ . Both MITE and MATE can be expressed as subsets of the unit sphere in  $\mathcal{H}_{\text{mc}}$ ,

$$\mathbb{S}(\mathcal{H}_{\text{mc}}) = \{\psi \in \mathcal{H}_{\text{mc}} : \|\psi\| = 1\}. \quad (1)$$

We define them in Sections 2 and 3, respectively, and discuss the properties and differences of the two notions in Section 4. We also note there that these notions can also be applied to mixed states.

## 2 MATE

The definition of MATE is based on macro observables  $\hat{M}_1, \dots, \hat{M}_K$ . These can be based on a partition of the system's available volume  $\Lambda \subset \mathbb{R}^3$  into cells  $\Lambda_i$  that are small on the macro scale but still large enough to each contain a large number of degrees of freedom. Examples of natural choices of  $\hat{M}$ 's are, for each cell, the number of particles of each type, the total energy, the total momentum, and/or the total magnetization.

Following von Neumann [45], we take the  $\hat{M}_j$  to commute with each other and to be such that the gaps between the eigenvalues are of the order of the macroscopic resolution (so that the eigenvalues are highly degenerate). This can be achieved by suitably “rounding off” and coarse-graining the operators representing the macro observables [45, 16, 25]. Taking  $\mathcal{H}_{\text{mc}}$  to be an eigenspace of a “macro energy” operator, and thus to commute with the other macro observables, all  $\hat{M}_j$  can be regarded as operators on  $\mathcal{H}_{\text{mc}}$ . Their joint spectral decomposition defines an orthogonal decomposition

$$\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_{\nu}, \quad (2)$$

and the subspaces  $\mathcal{H}_{\nu}$  (“macro spaces”), the joint eigenspaces of the macro observables, correspond to the different macro states and have very high dimension [17, 20, 14]. It is generally the case that one of the  $\mathcal{H}_{\nu}$ , denoted  $\mathcal{H}_{\text{eq}}$ , has most of the dimensions of  $\mathcal{H}_{\text{mc}}$ , i.e.,

$$\frac{\dim \mathcal{H}_{\text{eq}}}{\dim \mathcal{H}_{\text{mc}}} = 1 - \varepsilon \quad (3)$$

with  $\varepsilon \ll 1$ .<sup>1</sup> A realistic value for  $\varepsilon$ , say for a cubic meter of air at room conditions, is less than  $10^{-10^6}$  (see Supplementary Note); more generally,  $\varepsilon$  is exponentially small in the number of degrees of freedom per cell. We assume here that our system and our choice of macro observables are such that (3) holds for suitably small  $\varepsilon$ .

The system is said to be in *MATE* whenever its wave function  $\psi$  lies in the set

$$\text{MATE} = \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_{\text{eq}} | \psi \rangle > 1 - \delta \right\}, \quad \delta \ll 1, \quad (4)$$

with  $\hat{P}_{\text{eq}}$  the projection to  $\mathcal{H}_{\text{eq}}$ . Thus for a state  $\psi$  that is in MATE, the probability is close to one that all macro observables take on their thermal equilibrium values. A concept of thermal equilibrium along these lines was used before in, e.g., [17, 33, 14, 10, 11, 12]. It is known [14] that, if  $\varepsilon \ll \delta$ , then MATE has most of the surface area of  $\mathbb{S}(\mathcal{H}_{\text{mc}})$ , so most pure states are in MATE (see Section 4). It can also be shown, see (12) below, that most energy eigenstates are in MATE. To be sure, there are states in the energy shell which are not in MATE; for example, one could take a tensor product of states of two regions having (what look macroscopically like) different temperatures.

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<sup>1</sup>An exception to the existence of a dominant macro space is provided by first-order phase transitions, such as in the ferromagnetic Ising model in a vanishing external magnetic field, where  $\mathcal{H}_{\nu}$  has the appropriate majority of spins up and  $\mathcal{H}_{\nu'}$  has the appropriate majority of spins down, each having nearly 50% of the dimension of  $\mathcal{H}_{\text{mc}}$  for a suitable energy interval.

An alternative definition due to Tasaki [43, 44] (in the same direction as [5, 41]), not strictly but approximately equivalent and denoted TMATE here, avoids the step of rounding off to make the macro observables commute, which may pose substantial difficulty to carry out in practice. Instead, take  $\hat{M}_1, \dots, \hat{M}_K$  to be the macro observables before rounding off and coarse graining (mathematically, any self-adjoint operators), let  $V_j = \text{tr}(\hat{\rho}^{\text{mc}} \hat{M}_j)$  be the thermal equilibrium value of  $\hat{M}_j$ , and let  $\Delta M_j$  be the macro resolution of the observable represented by  $\hat{M}_j$ . Using  $1_A$  to denote the characteristic function of the set  $A$ , we define

$$\hat{P}_j = 1_{[V_j - \Delta M_j, V_j + \Delta M_j]}(\hat{M}_j) \quad (5)$$

to be the projection associated with the eigenvalues of  $\hat{M}_j$  that lie within the macro resolution of the thermal equilibrium value. Then let

$$\text{TMATE} = \bigcap_{j=1}^K \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_j | \psi \rangle > 1 - \delta \right\}. \quad (6)$$

Note that  $\langle \psi | \hat{P}_j | \psi \rangle$  is the probability of finding, in a quantum measurement of  $\hat{M}_j$  on a system in state  $\psi$ , a value that is  $\Delta M_j$ -close to  $V_j$ . If this probability is  $> 1 - \delta$  for at least the fraction  $1 - \eta$  of  $\mathbb{S}(\mathcal{H}_{\text{mc}})$  for each  $j$ , then TMATE has at least size  $1 - K\eta$  (in terms of normalized surface area), which is close to 1 if  $\eta \ll K^{-1}$ . We note further that MATE as in (4) can essentially also be written as the right-hand side of (6) if the  $\hat{M}_j$  are taken again as commuting and coarse-grained on the scale  $\Delta M_j$ .

### 3 MITE

While MATE implies thermal behavior only for macro observables, MITE involves also “micro” observables, more precisely, those observables concerning only a region smaller than a certain length scale  $\ell$ . The definition of MITE is inspired by *canonical typicality*, the observation [7, 27, 28, 15] that for any not-too-large subsystem  $S$  and most wave functions  $\psi$  in the energy shell  $\mathcal{H}_{\text{mc}}$ , the reduced density matrix of  $S$  is close to the thermal equilibrium density matrix of  $S$ ,  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}}$ , where  $\hat{\rho}_S^\psi = \text{tr}_{S^c} |\psi\rangle\langle\psi|$  is the reduced density matrix of  $S$  obtained by tracing out the complement  $S^c$  of  $S$ , and  $\hat{\rho}_S^{\text{mc}} = \text{tr}_{S^c} \hat{\rho}^{\text{mc}}$ . If  $S$  is small enough then  $\hat{\rho}_S^{\text{mc}} \approx \hat{\rho}_S^{(\beta)}$  for suitable  $\beta > 0$ , where the right-hand side is the partial trace,  $\hat{\rho}_S^{(\beta)} = \text{tr}_{S^c} \hat{\rho}^{(\beta)}$ , of the canonical density matrix  $\hat{\rho}^{(\beta)} = \frac{1}{Z} e^{-\beta \hat{H}}$  with  $Z = \text{tr} e^{-\beta \hat{H}}$ . As a consequence, for small  $S$ ,  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{(\beta)}$ . Hence, it does not matter whether one starts from  $\hat{\rho}^{\text{mc}}$  or  $\hat{\rho}^{(\beta)}$  (this fact is a version of equivalence of ensembles), and we will call either one the canonical or thermal density matrix for  $S$ .<sup>2</sup> We note that

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<sup>2</sup>The density matrix  $Z_S^{-1} \exp(-\beta \hat{H}_S)$  with  $\hat{H}_S$  the Hamiltonian of  $S$  is sometimes called the canonical or thermal density matrix for  $S$ ; it agrees with  $\hat{\rho}_S^{(\beta)}$  if the interaction between  $S$  and its complement can be neglected. If the interaction cannot be neglected, then  $\hat{\rho}_S^{(\beta)}$  is the correct density matrix to use.

if  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}}$  for some subsystem  $S$  then the same is true for every smaller subsystem  $S'$  contained in  $S$  (“subsubsystem property”), just by taking another partial trace on both sides of the approximate equation  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}}$ .

The system is said to be in  $\text{MITE}_\ell$  (MITE on the length scale  $\ell$ ) whenever its wave function  $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$  satisfies  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}}$  for every subsystem  $S$  corresponding to a spatial region of diameter  $\text{diam}(S) \leq \ell$ , i.e.,

$$\text{MITE}_\ell = \bigcap_{S : \text{diam}(S) \leq \ell} \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}} \right\} \quad (7)$$

with some precise definition of  $\approx$  (such as the trace norm of the difference being smaller than a given value). The subsubsystem property implies that every  $\psi$  in  $\text{MITE}_\ell$  lies also in  $\text{MITE}_{\ell'}$  for any smaller scale  $0 < \ell' < \ell$ .

*MITE* is then defined to mean  $\text{MITE}_{\ell_0}$  with  $\ell_0$  the largest  $\ell$  small enough to ensure that  $\hat{\rho}_S^{\text{mc}} \approx \hat{\rho}_S^{(\beta)}$  for every subsystem  $S$  with  $\text{diam}(S) \leq \ell_0$ . As a practical value, for example, we may take  $\ell_0 = 10^{-3} \text{diam}(\Lambda)$ , where  $\Lambda \subset \mathbb{R}^3$  is the volume of the whole system. Thus a state  $\psi$  is in *MITE* if for every subsystem of diameter  $\ell_0$  or smaller, the reduced density matrix is close to the thermal equilibrium reduced density matrix.

Most  $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$  lie in *MITE*. Indeed, canonical typicality (in the sense of  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}}$  for most  $\psi$ ) holds for subsystems of size up to nearly half that of  $\Lambda$  (that is, of half the total number of degrees of freedom, see Theorem 1 in [27]). We can choose a moderate number  $r$  (e.g.,  $r = 8$  for cube-shaped  $\Lambda$ ) of overlapping regions  $S_i \subset \Lambda$  (e.g., also cubes) of nearly half the volume so that most  $\psi$  satisfy  $\hat{\rho}_{S_i}^\psi \approx \hat{\rho}_{S_i}^{\text{mc}}$  for all  $1 \leq i \leq r$  simultaneously, and so that every region  $S$  with  $\text{diam}(S) \leq \frac{1}{4} \text{diam}(\Lambda)$  is contained in one of the  $S_i$ . By the subsubsystem property, also  $\hat{\rho}_S^\psi \approx \hat{\rho}_S^{\text{mc}}$  for such regions  $S$ , so most  $\psi$  lie in  $\text{MITE}_{\text{diam}(\Lambda)/4}$  and a fortiori in  $\text{MITE} = \text{MITE}_{\ell_0}$  with  $\ell_0$  as above.

A concept along the lines of *MITE* was used before in, e.g., [30, 21, 34, 23].

## 4 Discussion

*MITE implies MATE.*—For any observable  $\hat{A}$ , let  $\mu_{\hat{A}}^\psi$  denote the probability distribution defined by  $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$  over the spectrum of  $\hat{A}$ ,

$$\mu_{\hat{A}}^\psi(B) = \langle \psi | 1_B(\hat{A}) | \psi \rangle \quad (8)$$

for all sets  $B \subseteq \mathbb{R}$  (with  $1_B(\hat{A})$  the projection to the subspace spanned by the eigenvectors of  $\hat{A}$  with eigenvalue in  $B$ ). Likewise, let  $\mu_{\hat{A}}^{\text{mc}}$  denote the probability distribution defined by the micro-canonical ensemble,

$$\mu_{\hat{A}}^{\text{mc}}(B) = \text{tr}(1_B(\hat{A}) \hat{\rho}^{\text{mc}}) \quad (9)$$

for all  $B \subseteq \mathbb{R}$ ;  $\mu_{\hat{A}}^{\text{mc}}$  is the average of  $\mu_{\hat{A}}^\psi$  with  $\psi$  taken to be uniformly distributed in  $\mathbb{S}(\mathcal{H}_{\text{mc}})$ .

Both MITE and MATE are ultimately of the following form (see also [41]): For a certain family  $\mathcal{A}$  of observables, consider the set of  $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$  for which  $\mu_{\hat{A}}^{\psi} \approx \mu_{\hat{A}}^{\text{mc}}$  for all  $\hat{A} \in \mathcal{A}$ . MATE is obtained by taking  $\mathcal{A} = \mathcal{A}_{\text{MATE}} = \{\hat{M}_1, \dots, \hat{M}_K\}$ , and MITE $_{\ell}$  by taking  $\mathcal{A} = \mathcal{A}_{\text{MITE}_{\ell}} = \cup_S \mathcal{A}_S$  with the union taken over all regions in  $\Lambda$  of diameter  $\leq \ell$  and  $\mathcal{A}_S$  the set of *all* self-adjoint operators on  $\mathcal{H}_S$ , more precisely,

$$\mathcal{A}_S = \{ \hat{A}_0 \otimes \hat{I}_{S^c} : \hat{A}_0 \text{ self-adjoint on } \mathcal{H}_S \}, \quad (10)$$

where  $\hat{I}$  denotes the identity operator and  $S^c$  again the complement of  $S$ . Indeed, for  $\hat{A} = \hat{A}_0 \otimes \hat{I}_{S^c}$  and  $\psi \in \text{MITE}_{\ell}$ ,

$$\mu_{\hat{A}}^{\text{mc}}(B) = \text{tr}(1_B(\hat{A}) \hat{\rho}^{\text{mc}}) = \text{tr}(1_B(\hat{A}_0) \hat{\rho}_S^{\text{mc}}) \approx \text{tr}(1_B(\hat{A}_0) \hat{\rho}_S^{\psi}) = \mu_{\hat{A}}^{\psi}(B) \quad (11)$$

for all  $B \subseteq \mathbb{R}$  by (7).

From this perspective it is obvious that MITE implies MATE when based on reasonable choices: Suppose that  $L \leq \ell_0$ , where  $L$  is the length scale of the macro observables—the diameter of the cells  $\Lambda_i$  on which the macro observables  $\hat{M}_j$  were defined at the beginning of Section 2; that is, suppose that  $\hat{\rho}_S^{\psi} \approx \hat{\rho}_S^{\text{mc}}$  at least up to the length scale of the macro observables. This is commonly the case; e.g., for a cubic meter of gas at room conditions, we can realistically take  $L \approx 10^{-4}$  m and  $\ell_0 \approx 10^{-3}$  m. As a consequence of  $L \leq \ell_0$ ,  $\mathcal{A}_{\text{MATE}} \subset \mathcal{A}_{\text{MITE}}$ , so if  $\psi \in \text{MITE}$  then  $\psi \in \text{MATE}$ .

As a simple example of a state in MATE that is not in MITE, consider  $N \gg 1$  spins,  $\mathcal{H} = (\mathbb{C}^2)^{\otimes N}$ , Hamiltonian  $\hat{H} = 0$ ,  $\mathcal{H}_{\text{mc}} = \mathcal{H}$ , so  $\hat{\rho}^{\text{mc}} = 2^{-N} \hat{I}$ ; choose  $X_1, \dots, X_N \in \{-1, +1\}$  at random independently with equal probabilities, and let  $\psi = \phi_{X_1} \otimes \dots \otimes \phi_{X_N}$  with  $\phi_{\pm 1} = |\sigma_z = \pm 1\rangle$ . Then it is easy to see that most such  $\psi$ 's are in MATE, defined appropriately in terms of the macro-observables describing all components of the total magnetization of the cells  $\Lambda_i$ . However, for  $S$  any subsystem consisting of a single spin,  $\hat{\rho}_S^{\psi} = |\phi_{X_i}\rangle\langle\phi_{X_i}| \neq \hat{\rho}_S^{\text{mc}} = \hat{I}_S/2$ , so  $\psi$  is not in MITE. This example is very similar to a typical eigenstate of a system with MBL [18, 35, 23].

*ETH.*—To come back to the eigenstate thermalization hypothesis (ETH), it comes in two variants: MATE-ETH and a more refined version MITE-ETH, according to whether the energy eigenstates are required to be in MATE or MITE. It is MITE-ETH that fails dramatically in some MBL systems, according to the findings of [2, 26, 18]; there it is shown for certain MBL systems that a substantial fraction of the energy eigenstates (in a micro-canonical energy interval), or even all of them, lie outside of MITE. At the same time, it is easy to see that for every macroscopic quantum system (MBL or not), MATE-ETH must be almost satisfied, in the sense that most energy eigenstates  $|n\rangle \in \mathbb{S}(\mathcal{H}_{\text{mc}})$  are in MATE: Assuming that (3) holds with  $\varepsilon \ll \delta$ , we obtain, writing  $D = \dim \mathcal{H}_{\text{mc}}$ , that

$$\frac{1}{D} \sum_{n=1}^D \langle n | \hat{P}_{\text{eq}} | n \rangle = \frac{1}{D} \text{tr}(\hat{P}_{\text{eq}}) = 1 - \varepsilon, \quad (12)$$

and since  $\langle n | \hat{P}_{\text{eq}} | n \rangle$  cannot exceed 1, most of these terms must be close to 1.

If MATE-ETH holds strictly, i.e., if *all* energy eigenstates in  $\mathcal{H}_{\text{mc}}$  are in MATE, then every state  $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$  will sooner or later reach MATE and spend most of the time in MATE in the long run. That is because [14], writing  $\overline{f(t)} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(t) dt$  for time averages,  $|n\rangle$  for the energy eigenstate with eigenvalue  $E_n$ , and  $\psi_t = e^{-i\hat{H}t}\psi$ ,

$$\overline{\langle \psi_t | \hat{P}_{\text{eq}} | \psi_t \rangle} = \sum_{n, n'} \langle \psi | n \rangle \overline{e^{iE_n t} \langle n | \hat{P}_{\text{eq}} | n' \rangle e^{-iE_{n'} t}} \langle n' | \psi \rangle \quad (13)$$

$$= \sum_n |\langle \psi | n \rangle|^2 \langle n | \hat{P}_{\text{eq}} | n \rangle \geq \sum_n |\langle \psi | n \rangle|^2 (1 - \delta) = 1 - \delta, \quad (14)$$

provided  $\hat{H}$  is non-degenerate, i.e.,  $E_n \neq E_{n'}$  for  $n \neq n'$  (using  $\overline{e^{iEt}} = 1$  if  $E = 0$  and  $= 0$  otherwise).<sup>3</sup> Since its time average is close to 1,  $\langle \psi_t | \hat{P}_{\text{eq}} | \psi_t \rangle$  must be close to 1 for most  $t$  in the long run.

It follows from this that systems with MBL for which the transport coefficients vanish, so that an initial state  $\psi$  with a non-uniform temperature will remain so indefinitely, cannot have all of its energy eigenfunctions in MATE. Since most energy eigenstates are in MATE, such  $\psi$  must be a superposition of predominantly those rare eigenstates that are not in MATE.

This leads to the question whether there are macroscopic systems for which *all* energy eigenstates are in MATE—i.e., whether MATE-ETH ever strictly holds. It is known that this is so for a random Hamiltonian whose eigenbasis is uniformly chosen among all orthonormal bases [14]; see also [45, 16]. Some numerical evidence [19] points to the existence of systems with realistic interactions for which all energy eigenstates are in MATE and thus also in MATE.

For MITE-ETH, there are several results [33, 21, 31], one of which [33] is based on Srednicki's [39, 40] extension of the ETH to off-diagonal elements.

*Mixed states.*—Once we have the notions of MITE and MATE for pure states  $\psi$ , they are easily generalized to mixed states  $\hat{\rho}$ : MATE occurs if  $\text{tr}(\hat{P}_{\text{eq}} \hat{\rho}) > 1 - \delta$ , and MITE if  $\hat{\rho}_S \approx \hat{\rho}_S^{\text{mc}}$  for all subsystems  $S$  defined by spatial regions of diameter  $\leq \ell_0$ . Note that neither MATE nor MITE requires that  $\hat{\rho}$  be close to  $\hat{\rho}^{\text{mc}}$  or  $\hat{\rho}^{(\beta)}$ .

*Thermal equilibrium in classical mechanics.*—Only one of the two notions MITE and MATE can be satisfied for pure states in classical mechanics, namely MATE. That is because a “pure state” corresponds in classical mechanics to a point  $X$  in phase space, while a “mixed state” corresponds to a probability distribution over phase space. Since  $X$  specifies the positions and momenta of all particles, it also provides a pure state for any subsystem. In contrast, in quantum mechanics  $\hat{\rho}_S^\psi$  can be mixed, and in fact is mixed except for product states. So in classical mechanics it is never true for a system in a pure state that a subsystem  $S$  could have a state close to a thermodynamic ensemble such as the marginal (obtained by integrating out the variables not belonging to  $S$ ) of the

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<sup>3</sup>In fact, the assumption of non-degeneracy can be dropped: If we number the eigenvalues as  $E_n$  with  $E_n \neq E_{n'}$  for  $n \neq n'$  and let  $|n\rangle$  denote the normalized projection of  $\psi$  to the eigenspace of  $E_n$ , then the calculation (13)–(14) still applies.

micro-canonical distribution (i.e., uniform over the energy shell) or the canonical one for the whole system. In contrast, MATE is analogous to Boltzmann’s [4, 9, 13, 20] notion of thermal equilibrium for a closed classical system, based on a partition of phase space into macro states  $\Gamma_\nu$ . (Note that there is no difference between MATE and TMATE classically, as all observables commute.)

## 5 Conclusions

Perhaps the most surprising aspect of the situation is that the various criteria for thermal equilibrium of pure states proposed in the literature fall into two groups that differ substantially in how much they demand.

Arguably, the essence of thermal equilibrium is what characterizes it in thermodynamics: that a system appears stationary on the macro level, and that temperature and all chemical potentials are spatially uniform. This corresponds to MATE, which may therefore be regarded as the direct expression of thermal equilibrium. On the other hand, since MITE is the stronger statement, and since it is usually true that macroscopic quantum systems approach MITE (MBL systems being an exception), it is natural to consider MITE, and it would seem artificial to not regard it as a new kind of thermal equilibrium property emerging from quantum entanglement.

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## 6 Supplementary Note

Here is a simple reasoning leading to this value of  $\varepsilon$ . Suppose we partition the cubic meter 3-volume  $\Lambda \subset \mathbb{R}^3$  of this macroscopic gas into  $n$  (say,  $10^{12}$ ) cells  $\Lambda_j$  of equal volume and take the macro variable  $\hat{M}_j$  to be the number of molecules  $\hat{N}_j$  in  $\Lambda_j$ , divided by the total number  $N$  and coarse grained with resolution  $\Delta M_j$  (say,  $\Delta M_j = 10^{-3}/n$ ). For simplicity, we leave aside considerations of energy and estimate  $\varepsilon$  by means of a uniform probability distribution over  $\Lambda^N$  and the corresponding joint distribution of the  $M_j$ . Clearly,  $M_j$  has equilibrium value  $\nu_j^{\text{eq}} = 1/n$  (and the relative resolution is  $\Delta M_j/\nu_j^{\text{eq}} = 10^{-3}$ ); the distribution of  $N_j$  is binomial with parameters  $N$  and  $1/n$  and thus, if  $N/n$  is large, approximately Gaussian with parameters  $\mu = N/n$  and  $\sigma^2 \approx N/n$ . For  $M_j$  to deviate from its equilibrium value requires that  $N_j$  deviates from  $\mu$  by more than  $N \Delta M_j$ , i.e., by more than  $\sqrt{nN} \Delta M_j$  standard deviations, which has probability less than  $p := \exp(-nN \Delta M_j^2)$ . Since the  $N_j$  are approximately independent, the probability that *any* of the  $M_j$  deviates from its equilibrium value is  $np$ , which here is still of rough order of magnitude  $\exp(-10^{-6}(N/n))$ . The cells we consider are of volume  $10^{-12} \text{ m}^3$  and at standard (room) conditions contain more than  $10^{13}$  molecules, giving  $\varepsilon < 10^{-10^6}$ .