Approach to thermal equilibrium of macroscopic quantum systems

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We consider an isolated macroscopic quantum system. Let $\mathcal{H}$ be a microcanonical "energy shell," i.e., a subspace of the system's Hilbert space spanned by the (finitely) many energy eigenstates with energies between E and $E+\delta E$. The thermal equilibrium macrostate at energy E corresponds to a subspace $\mathcal{H}_{eq}$ of $\mathcal{H}$ such that $\dim \mathcal{H}_{eq}/\dim \mathcal{H}$ is close to 1. We say that a system with state vector $\psi \in \mathcal{H}$ is in thermal equilibrium if ψ is "close" to $\mathcal{H}_{eq}$. We show that for "typical" Hamiltonians with given eigenvalues, all initial state vectors ψ_0 evolve in such a way that ψ_t is in thermal equilibrium for most times t. This result is closely related to von Neumann's quantum ergodic theorem of 1929.

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I. INTRODUCTION

If a hot brick is brought in contact with a cold brick, and the two bricks are otherwise isolated, then energy will flow from the hot to the cold brick until their temperatures become equal, i.e., the system equilibrates. Since the bricks ultimately consist of electrons and nuclei, they form a quantum system with a huge number ($>10^{20}$) of particles; this is an example of an *isolated macroscopic quantum system*.

From a microscopic point of view the state of the system at time t is described by a vector

$$\psi(t) = e^{-iHt}\psi(0) \tag{1}$$

in the system's Hilbert space or a density matrix

$$\rho(t) = e^{-iHt}\rho(0)e^{iHt}, \tag{2}$$

where H is the Hamiltonian of the isolated system and we have set $\hbar = 1$. In this paper we prove a theorem asserting that for a sufficiently large quantum system with a typical Hamiltonian and an *arbitrary initial state* $\psi(0)$, the system's state $\psi(t)$ spends most of the time, in the long run, in thermal equilibrium. (Of course, before the system even reaches thermal equilibrium there could be a waiting time longer than the present age of the universe.) This implies the same behavior for an arbitrary $\rho(0)$.

This behavior of isolated macroscopic quantum systems is an instance of a phenomenon we call *normal typicality* [1], a version of which is expressed in von Neumann's quantum ergodic theorem [2]. However, our result falls outside the scope of von Neumann's theorem because of the technical assumptions made in that theorem. Our result also differs from the related results in [3–8], which use different notions of when a system is in an equilibrium state. In particular they do not regard the thermal equilibrium of an isolated macroscopic system as corresponding to its wave function being close to a subspace $\mathcal{H}_{eq}$ of Hilbert space. See Sec. VI for further discussion.

The rest of this paper is organized as follows. In the remainder of Sec. I, we define more precisely what we mean by thermal equilibrium. In Sec. II we outline the problem and our result, Theorem 1. In Sec. III we prove the key estimate for the proof of Theorem 1. In Sec. IV we describe examples of exceptional Hamiltonians, illustrating how a system can fail to ever approach thermal equilibrium. In Sec. V we compare our result to the situation with classical systems. In Sec. VI we discuss related works.

A. Equilibrium subspace

Let $\mathcal{H}_{\text{total}}$ be the Hilbert space of a macroscopic system in a box Λ, and let H be its Hamiltonian. Let $\{\phi_\alpha\}$ be an orthonormal basis of $\mathcal{H}_{\text{total}}$ consisting of eigenvectors of H with eigenvalues E_α. Consider an energy interval $[E, E+\delta E]$, where δE is small on the macroscopic scale but large enough for the interval $[E, E+\delta E]$ to contain very many eigenvalues. Let $\mathcal{H} \subseteq \mathcal{H}_{\text{total}}$ be the corresponding subspace,

$$\mathcal{H} = \text{span}\{\phi_\alpha : E_\alpha \in [E, E+\delta E]\}. \tag{3}$$

A subspace such as $\mathcal{H}$ is often called a *microcanonical energy shell*. Let D be the dimension of $\mathcal{H}$, i.e., the number of energy levels, including multiplicities, between E and $E+\delta E$. In the following we consider only quantum states ψ that lie in $\mathcal{H}$, i.e., of the form

$$\psi = \sum_\alpha c_\alpha \phi_\alpha \tag{4}$$

with $c_\alpha \neq 0$ only for α such that $E_\alpha \in [E, E+\delta E]$.

According to the analysis of von Neumann [2,9] and others (cf. [10]), the macroscopic (coarse-grained) observables in a macroscopic quantum system can be naturally "rounded" to form a set of commuting operators,

$$\{M_i\}_{i=1,\ldots,k}. \tag{5}$$

The operators are defined on $\mathcal{H}_{\text{total}}$, but since we can take them to include (and thus commute with) a coarse-grained

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Hamiltonian, we can (and will) take them to commute with the projection to $\mathcal{H}$, and thus to map $\mathcal{H}$ to itself. We write $\nu=(m_1,\ldots,m_k)$ for a list of eigenvalues m_i of the restriction of M_i to $\mathcal{H}$, and $\mathcal{H}_\nu$ for the joint eigenspace. Such a set of operators generates an orthogonal decomposition of the Hilbert space

$$\mathcal{H}=\bigoplus_\nu \mathcal{H}_\nu, \tag{6}$$

where each $\mathcal{H}_\nu$, called a macrospace, represents a macrostate of the system. The dimension of $\mathcal{H}_\nu$ is denoted by d_ν; note that $\Sigma_\nu d_\nu=D$. If any $\mathcal{H}_\nu$ has a dimension of zero, we remove it from the family $\{\mathcal{H}_\nu\}$. In practice, $d_\nu \gg 1$, since we are considering a macroscopic system with coarse-grained observables.

It can be shown in many cases, and is expected to be true generally, that among the macrospaces $\mathcal{H}_\nu$ there is a particular macrospace $\mathcal{H}_{eq}$, the one corresponding to thermal equilibrium, such that

$$d_{eq}/D \approx 1, \tag{7}$$

indeed with the difference $1-d_{eq}/D$ exponentially small in the number of particles.[1] This implies, in particular, that each of the macro-observables M_i is "nearly constant" on the energy shell $\mathcal{H}$ in the sense that one of its eigenvalues has multiplicity at least $d_{eq}\approx D$. We say that a system with quantum state ψ (with $\|\psi\|=1$) is *in thermal equilibrium* if ψ is very close (in the Hilbert space norm) to $\mathcal{H}_{eq}$, i.e., if

$$\langle\psi|P_{eq}|\psi\rangle \approx 1, \tag{8}$$

where P_{eq} is the projection operator to $\mathcal{H}_{eq}$. The corresponding relation for density matrices is

$$\mathrm{Tr}(P_{eq}\rho) \approx 1. \tag{9}$$

Condition (8) implies that a quantum measurement of the macroscopic observable M_i on a system with wave function ψ will yield, with probability close to 1, the "equilibrium" value of M_i. Likewise, a joint measurement of $M_1,\ldots,M_k$ will yield, with probability close to 1, their equilibrium values.

Let $\mu(d\psi)$ be the uniform measure on the unit sphere in $\mathcal{H}$ [12,13]. It follows from Eq. (7) that most ψ relative to μ are in thermal equilibrium. Indeed,

$$\int \langle\psi|P_{eq}|\psi\rangle\mu(d\psi)=\frac{1}{D}\mathrm{Tr}\ P_{eq}=\frac{d_{eq}}{D}\approx 1. \tag{10}$$

Since the quantity $\langle\psi|P_{eq}|\psi\rangle$ is bounded from above by 1, most ψ must satisfy Eq. (8).[2]

B. Examples of equilibrium subspaces

To illustrate the decomposition into macrostates, we describe two examples. As example 1, consider a system composed of two identical subsystems designated 1 and 2, e.g., the bricks mentioned in the beginning of this paper, with Hilbert space $\mathcal{H}_{\mathrm{total}}=\mathcal{H}_1\otimes\mathcal{H}_2$. The Hamiltonian of the total system is

$$H=H_1+H_2+\lambda V, \tag{11}$$

where H_1 and H_2 are the Hamiltonians of subsystems 1 and 2, respectively, and λV is a small interaction between the two subsystems. We assume that H_1, H_2, and H are positive operators. Let $\mathcal{H}$ be spanned by the eigenfunctions of H with energies between E and $E+\delta E$.

In this example, we consider just a single macro-observable M, which is a projected and coarse-grained version of H_1/E, i.e., of the fraction of the energy that is contained in subsystem 1 alone. We cannot take M to simply equal to H_1/E because H_1 is defined on $\mathcal{H}_{\mathrm{total}}$, not $\mathcal{H}$, and will generically not map $\mathcal{H}$ to itself, while we would like M to be an operator on $\mathcal{H}$. To obtain an operator on $\mathcal{H}$, let P be the projection $\mathcal{H}_{\mathrm{total}}\to\mathcal{H}$ and set

$$H_1'=PH_1P \tag{12}$$

(more precisely, H_1' is PH_1 restricted to $\mathcal{H}$). Note that H_1' is a positive operator, but might have eigenvalues greater than E. Now define[3]

$$M=f(H_1'/E) \tag{13}$$

with the coarse-graining function

$$f(x)=\begin{cases}0 & \text{if } x<0.01\\ 0.02 & \text{if } x\in[0.01,0.03)\\ 0.04 & \text{if } x\in[0.03,0.05)\\ \text{etc.} & \ldots.\end{cases} \tag{14}$$

$\mathcal{H}_\nu$ are the eigenspaces of M; clearly, $\oplus_\nu\mathcal{H}_\nu=\mathcal{H}$. If, as we assume, λV is small, then we expect $\mathcal{H}_{0.5}=\mathcal{H}_{eq}$ to have the overwhelming majority of dimensions. In a thorough treatment we would need to prove this claim, as well as that H_1' is not too different from H_1, but we do not give such a treatment here.

As example 2, consider N bosons (fermions) in a box $\Lambda=[0,L]^3\subseteq\mathbb{R}^3$; i.e., $\mathcal{H}_{\mathrm{total}}$ consists of the square-integrable (anti)symmetric functions on Λ^N. Let the Hamiltonian be

[1] This dominance of the equilibrium state can be expressed in terms of the (Boltzmann) entropy S_ν of a macroscopic system in the macrostate ν, be it the equilibrium state or some other (see [11]), defined as $S_\nu=k_B\log d_\nu$, where k_B is the Boltzmann constant: d_{eq}/D being close to 1 just expresses the fact that the entropy of the equilibrium state is close to the microcanonical entropy S_{mc}, i.e., $S_{eq}=k_B\log d_{eq}\approx k_B\log D=S_{mc}$.

[2] It should in fact be true for a large class of observables A on $\mathcal{H}$ that, for most ψ relative to μ, $\langle\psi|A|\psi\rangle\approx\mathrm{Tr}(\rho_{mc}A)$, where ρ_{mc} is the microcanonical density matrix, i.e., $1/D$ times the identity on $\mathcal{H}$. This is relevant to the various results on thermalization described in Sec. VI.

[3] Recall that the application of a function f to a self-adjoint matrix A is defined to be $f(A)=\Sigma f(a_\alpha)|\varphi_\alpha\rangle\langle\varphi_\alpha|$ if the spectral decomposition of A reads $A=\Sigma a_\alpha|\varphi_\alpha\rangle\langle\varphi_\alpha|$.

$$H = -\frac{1}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} v(|\boldsymbol{q}_i - \boldsymbol{q}_j|), \tag{15}$$

where the Laplacian ∇_i^2 has Dirichlet boundary conditions, $v(r)$ is a given pair potential, and $\boldsymbol{q}_i$ is the triple of position coordinates of the ith particle. Let $\mathcal{H}$ again be spanned by the eigenfunctions with energies between E and $E+\delta E$.

In this example, we consider again a single macro-observable M, based on the operator N_{left} for the number of particles in the left half of the box Λ,

$$N_{\text{left}}\psi(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N) = \#\{i:\boldsymbol{q}_i \in [0,L/2]\times[0,L]^2\}\psi(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N). \tag{16}$$

Note that the spectrum of N_{left} consists of the $N+1$ eigenvalues $0,1,2,\ldots,N$. To obtain an operator on $\mathcal{H}$, let P be the projection $\mathcal{H}_{\text{total}} \to \mathcal{H}$ and set $N'_{\text{left}} = PN_{\text{left}}P$. Note that the spectrum of N'_{left} is still contained in $[0,N]$. Now define $M = f(N'_{\text{left}}/N)$ with the coarse-graining function (14). We expect that for large N, the eigenspace with an eigenvalue of 0.5, $\mathcal{H}_{eq} = \mathcal{H}_{0.5}$, has the overwhelming majority of dimensions (and that $N'_{\text{left}} \approx N_{\text{left}}$).

II. FORMULATION OF PROBLEM AND RESULTS

Our goal is to show that, for typical macroscopic quantum systems,

$$\langle\psi(t)|P_{eq}|\psi(t)\rangle \approx 1 \quad \text{for most } t. \tag{17}$$

To see this, we compute the time average of $\langle\psi(t)|P_{eq}|\psi(t)\rangle$. We denote the time average of a time-dependent quantity $f(t)$ by an overbar,

$$\overline{f(t)} = \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, f(t). \tag{18}$$

Since $\langle\psi(t)|P_{eq}|\psi(t)\rangle$ is always a real number between 0 and 1, it follows that if its time average is close to 1 then it must be close to 1 most of the time. Moreover, for μ-most $\psi(0)$, where μ is the uniform measure on the unit sphere of $\mathcal{H}$, $\psi(t)$ is in thermal equilibrium most of the time. This result follows from Fubini's theorem (which implies that taking the μ average commutes with taking the time average) and the unitary invariance of μ,

$$\int \overline{\langle\psi(t)|P_{eq}|\psi(t)\rangle}\mu(d\psi) = \overline{\int \langle\psi|e^{iHt}P_{eq}e^{-iHt}|\psi\rangle\mu(d\psi)}$$
$$= \int \langle\psi|P_{eq}|\psi\rangle\mu(d\psi) \approx 1. \tag{19}$$

That is, the ensemble average of the time average is near 1, so, for μ-most $\psi(0)$, the time average must be near 1, which implies our claim above. So the interesting question is about the behavior of exceptional $\psi(0)$, e.g., of systems which are not in thermal equilibrium at $t=0$. Do they ever go to thermal equilibrium?

As we will show, for many Hamiltonians statement (17) holds in fact for *all* $\psi(0) \in \mathcal{H}$. From now on, let H denote the restriction of the Hamiltonian to $\mathcal{H}$, and let $\phi_1, \ldots, \phi_D$ be an orthonormal basis of $\mathcal{H}$ consisting of eigenvectors of the Hamiltonian H with eigenvalues $E_1, \ldots, E_D$. If

$$\psi(0) = \sum_{\alpha=1}^{D} c_\alpha\phi_\alpha, \quad c_\alpha = \langle\phi_\alpha|\psi(0)\rangle, \tag{20}$$

then

$$\psi(t) = \sum_{\alpha=1}^{D} e^{-iE_\alpha t}c_\alpha\phi_\alpha. \tag{21}$$

Thus,

$$\overline{\langle\psi(t)|P_{eq}|\psi(t)\rangle} = \sum_{\alpha,\beta=1}^{D}\overline{e^{i(E_\alpha-E_\beta)t}}c_\alpha^* c_\beta\langle\phi_\alpha|P_{eq}|\phi_\beta\rangle. \tag{22}$$

If H is nondegenerate (which is the generic case) then $E_\alpha - E_\beta$ vanishes only for $\alpha=\beta$, so the time averaged exponential is $\delta_{\alpha\beta}$, and

$$\overline{\langle\psi(t)|P_{eq}|\psi(t)\rangle} = \sum_{\alpha=1}^{D}|c_\alpha|^2\langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle. \tag{23}$$

Thus, for the system to be in thermal equilibrium most of the time it is necessary and sufficient that the right-hand side of Eq. (23) is close to 1.

Now if an energy eigenstate ϕ_α is not itself in thermal equilibrium then when $\psi(0)=\phi_\alpha$ the system is never in thermal equilibrium since this state is stationary. Conversely, if we have that

$$\langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle \approx 1 \quad \text{for all } \alpha, \tag{24}$$

then the system will be in thermal equilibrium most of the time for all $\psi(0)$. This follows directly from Eq. (23) since the right-hand side of Eq. (23) is an average of $\langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle$. We show below that Eq. (24) is true for "most" Hamiltonians and, thus, for most Hamiltonians it is the case that every wave function spends most of the time in thermal equilibrium.

A. Main result

The measure of most we use is the following: for any given D (distinct) energy values $E_1, \ldots, E_D$, we consider the uniform distribution μ_{Ham} over all Hamiltonians with these eigenvalues. Choosing H at random with distribution μ_{Ham} is equivalent to choosing the eigenbasis $\{\phi_\alpha\}$ according to the uniform distribution μ_{ONB} over all orthonormal bases of $\mathcal{H}$, and setting $H = \Sigma_\alpha E_\alpha|\phi_\alpha\rangle\langle\phi_\alpha|$. The measure μ_{ONB} can be defined as follows: choosing a random basis according to μ_{ONB} amounts to choosing ϕ_1 according to the uniform distribution over the unit sphere in $\mathcal{H}$, then ϕ_2 according to the uniform distribution over the unit sphere in the orthogonal complement of ϕ_1, etc. Alternatively, μ_{ONB} can be defined in terms of the Haar measure $\mu_{\mathcal{U}(D)}$ on the group $\mathcal{U}(D)$ of unitary $D \times D$ matrices: any given orthonormal basis $\{\chi_\alpha\}$ of $\mathcal{H}$ defines a one-to-one correspondence between $\mathcal{U}(D)$ and the set of all orthonormal bases of $\mathcal{H}$, associating with the matrix $U = (U_{\alpha\beta}) \in \mathcal{U}(D)$ the basis

$$\phi_\alpha = \sum_{\beta=1}^{D} U_{\alpha\beta}\chi_\beta. \tag{25}$$

The image of the Haar measure under this correspondence is in fact independent of the choice of $\{\chi_\beta\}$ (because of the invariance of the Haar measure under right multiplication) and is μ_{ONB}.

Put differently, the ensemble μ_{Ham} of Hamiltonians can be obtained by starting from a given Hamiltonian H_0 on $\mathcal{H}$ (with distinct eigenvalues $E_1,\ldots,E_D$) and setting

$$H = UH_0U^{-1} \tag{26}$$

with U a random unitary matrix chosen according to the Haar measure. Note that, while considering different possible Hamiltonians H in $\mathcal{H}$, we keep $\mathcal{H}_{eq}$ fixed, although in practice it would often be reasonable to select $\mathcal{H}_{eq}$ in a way that depends on H (as we did in the examples of Sec. I B).

For our purpose it is convenient to choose the basis $\{\chi_\alpha\}$ in such a way that the first d_{eq} basis vectors lie in $\mathcal{H}_{eq}$ and the other ones are orthogonal to $\mathcal{H}_{eq}$. Then, we have that

$$\langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle = \sum_{\beta=1}^{d_{eq}} |U_{\alpha\beta}|^2 \tag{27}$$

with $U_{\alpha\beta}$ the unitary matrix satisfying Eq. (25).

We will show first, in Lemma 1, that for every $0<\varepsilon<1$, if D is sufficiently large and d_{eq}/D sufficiently close to 1, then most orthonormal bases $\{\phi_\alpha\}$ are such that

$$\langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle > 1-\varepsilon \quad \text{for all } \alpha. \tag{28}$$

This inequality is a precise version of Eq. (24). How close to 1 should d_{eq}/D be? The fact that the average of $\langle\psi|P_{eq}|\psi\rangle$ over all wave functions ψ on the unit sphere of $\mathcal{H}$ equals d_{eq}/D, mentioned already in Eq. (10), implies that Eq. (28) cannot be true for most orthonormal bases if $d_{eq}/D \leq 1-\varepsilon$. To have enough wiggling room, we require that

$$\frac{d_{eq}}{D} > 1-\frac{\varepsilon}{2}. \tag{29}$$

We will show then, in Theorem 1, that for every (arbitrarily small) $0<\eta<1$ and for sufficiently large D, most H are such that for every initial wave function $\psi(0)\in\mathcal{H}$ with $\|\psi(0)\|=1$, the system will spend most of the time in thermal equilibrium with accuracy $1-\eta$, where we say that a system with wave function ψ is in thermal equilibrium with accuracy $1-\eta$ if

$$\langle\psi|P_{eq}|\psi\rangle > 1-\eta. \tag{30}$$

This inequality is a precise version of Eq. (8). In order to have no more exceptions in time than the fraction $0<\delta'<1$, we need to set ε in Eqs. (28) and (29) equal to $\eta\delta'$.

Lemma 1. Let $\mu_{\mathcal{U}(D)}$ denote the Haar measure on $\mathcal{U}(D)$, and

$$\mathcal{S}_\varepsilon := \left\{ U\in\mathcal{U}(D) \;\middle|\; \forall\,\alpha: \sum_{\beta=1}^{d_{eq}} |U_{\alpha\beta}|^2 > 1-\varepsilon \right\}. \tag{31}$$

Then for all $0<\varepsilon<1$ and $0<\delta<1$, there exists $D_0 = D_0(\varepsilon,\delta) > 0$ such that

$$\text{if } D>D_0, \quad d_{eq} > (1-\varepsilon/2)D \quad \text{then } \mu_{\mathcal{U}(D)}(\mathcal{S}_\varepsilon) \geq 1-\delta. \tag{32}$$

The proof of Lemma 1 is given in Sec. III. It also shows that D_0 can, for example, be chosen to be

$$D_0(\varepsilon,\delta) = \max[10^3\varepsilon^{-2}\log(4/\delta), 10^6\varepsilon^{-4}]. \tag{33}$$

Here and throughout this paper, log denotes the natural logarithm. From Eq. (27), we obtain

Theorem 1. For all $\eta,\delta,\delta'\in(0,1)$, all integers $D > D_0(\eta\delta',\delta)$ and all integers $d_{eq} > (1-\eta\delta'/2)D$ the following is true: let $\mathcal{H}$ be a Hilbert space of dimension D, let $\mathcal{H}_{eq}$ be a subspace of dimension d_{eq}, let P_{eq} denote the projection to $\mathcal{H}_{eq}$, let $E_1,\ldots,E_D$ be pairwise distinct but otherwise arbitrary, and choose a Hamiltonian at random with eigenvalues E_α and an eigenbasis ϕ_α that is uniformly distributed. Then, with probability at least $1-\delta$, every initial quantum state will spend $(1-\delta')$-most of the time in thermal equilibrium as defined in Eq. (30), i.e.,

$$\liminf_{T\to\infty} \frac{1}{T}\left|\{0<t<T:\langle\psi(t)|P_{eq}|\psi(t)\rangle > 1-\eta\}\right| \geq 1-\delta', \tag{34}$$

where $|M|$ denotes the size (Lebesgue measure) of the set M.

Proof. It follows from Lemma 1 that under the hypotheses of Theorem 1,

$$\overline{\langle\psi(t)|P_{eq}|\psi(t)\rangle} \geq 1-\eta\delta'$$

with probability at least $1-\delta$. Thus, since $\eta\delta' \geq \overline{1-\langle\psi(t)|P_{eq}|\psi(t)\rangle} \geq \eta\tilde{\delta}$, where $\tilde{\delta}$ is the $\limsup_{T\to\infty}$ of the fraction of the time in $(0,T)$ for which $\langle\psi(t)|P_{eq}|\psi(t)\rangle \leq 1-\eta$, it follows that $\tilde{\delta}\leq\delta'$. ■

B. Remarks

Normal typicality. Theorem 1 can be strengthened; with the same sense of "most" as in Theorem 1, we have that for most Hamiltonians and for all $\psi(0)$,

$$\langle\psi(t)|P_\nu|\psi(t)\rangle \approx \frac{\dim\mathcal{H}_\nu}{\dim\mathcal{H}}, \quad \text{for all } \nu, \tag{35}$$

for most t. For $\nu=eq$, this implies that $\langle\psi(t)|P_{eq}|\psi(t)\rangle\approx 1$. This stronger statement we have called normal typicality [1]. A version of normal typicality was proven by von Neumann [2]. However, because of the technical assumptions he made, von Neumann's result, while much more difficult, does not quite cover the simple result of this paper.

Typicality and probability. When we express that something is true for most H or most ψ relative to some normalized measure μ, it is often convenient to use the language of probability theory and speak of a random H or ψ chosen with distribution μ. However, by this we do not mean to imply that the actual H or ψ in a concrete physical situation is random, nor that one would obtain, in repetitions of the experiment or in a class of similar experiments, different H's or ψ's whose empirical distribution is close to μ. That would be a misinterpretation of the measure μ, one that suggests the

question whether perhaps the actual distribution in reality could be nonuniform. This question misses the point, as there need not be any actual distribution in reality. Rather, Theorem 1 means that the set of "bad" Hamiltonians has very small measure μ_{Ham}.

Consequences for example 2. From Lemma 1 it follows for example 2 that typical Hamiltonians of the form (26) with H_0 given by the right-hand side of Eq. (15) are such that all eigenfunctions are close to $\mathcal{H}_{0.5}$; this fact in turn strongly suggests (although we have not proved this) that the eigenfunctions are essentially concentrated on those configurations that have approximately 50% of the particles in the left half and 50% in the right half of the box.

Equilibrium statistical mechanics. Theorem 1 implies that, for typical H, every $\psi(0) \in \mathcal{H}$ is such that for most t,

$$\langle \psi(t)|M_i|\psi(t)\rangle \approx \mathrm{Tr}(\rho_{mc} M_i), \tag{36}$$

where ρ_{mc} is the standard microcanonical density matrix (i.e., $1/D$ times the projection $\mathcal{H}_{\mathrm{total}} \to \mathcal{H}$), for all macro-observables M_i as described in Sec. I A. This justifies replacing $|\psi(t)\rangle\langle\psi(t)|$ with ρ_{mc} as far as macro-observables in equilibrium are concerned. However, this does not—by itself—justify the use of ρ_{mc} for observables A not among $\{M_i\}$. For example, consider a microscopic observable A that is not "nearly constant" on the energy shell $\mathcal{H}$. Then, standard equilibrium statistical mechanics tells us to use ρ_{mc} for the expected value of A in equilibrium. We believe that this is in fact correct for most such observables, but it is not covered by Theorem 1. Results concerning many such observables are described in Sec. VI. These results, according to which, in an appropriate sense,

$$\langle \psi(t)|A|\psi(t)\rangle \approx \mathrm{Tr}(\rho_{mc} A) \tag{37}$$

for suitable A and $\psi(0)$, are valid only in quantum mechanics. The justification of the broad use of ρ_{mc} in classical statistical mechanics relies on rather different sorts of results requiring different kinds of considerations.

III. PROOF OF LEMMA 1

Proof. Let us write $\mathbb{P}$ for the Haar measure $\mu_{\mathcal{U}(D)}$, and let

$$p := \mathbb{P}\left(\bigcap_{\alpha=1}^{D}\left\{\sum_{\beta=1}^{d_{eq}} |U_{\alpha\beta}|^2 > 1-\varepsilon\right\}\right). \tag{38}$$

Observe that

$$p = 1 - \mathbb{P}\left(\bigcup_{\alpha=1}^{D}\left\{\sum_{\beta=1}^{d_{eq}} |U_{\alpha\beta}|^2 \le 1-\varepsilon\right\}\right) \tag{39}$$

$$\ge 1 - D \max_{\alpha} \mathbb{P}\left\{\sum_{\beta=1}^{d_{eq}} |U_{\alpha\beta}|^2 \le 1-\varepsilon\right\}. \tag{40}$$

Since $U=(U_{\alpha\beta})$ is a random unitary matrix with Haar distribution, its αth column is a random unit vector $\vec{U} := (U_{\alpha\beta})_\beta$ whose distribution is uniform over the unit sphere of $\mathbb{C}^D$ (i.e., the distribution is, up to a normalizing constant, the surface area measure). Therefore, the probability in the last line does not, in fact, depend on α, and so the step of taking the maximum over α can be omitted.

A random unit vector such as $\vec{U}$ can be thought of as arising from a random Gaussian vector $\vec{G}$ by normalization: let G_β for $\beta=1,\ldots,D$ be independent complex Gaussian random variables with mean zero and variance $\mathbb{E}|G_\beta|^2 = 1/D$; i.e., Re G_β and Im G_β are independent real Gaussian random variables with mean zero and variance $1/2D$. Then the distribution of $\vec{G}=(G_1,\ldots,G_D)$ is symmetric under rotations from $\mathcal{U}(D)$, and thus

$$\frac{\vec{G}}{\|\vec{G}\|} = \vec{U} \quad \text{in distribution,} \quad \text{with } \|\vec{G}\|^2 = \sum_{\beta=1}^{D} |G_\beta|^2. \tag{41}$$

We thus have that

$$p \ge 1 - D\mathbb{P}\left\{\sum_{\beta=1}^{d_{eq}} \frac{|G_\beta|^2}{\|\vec{G}\|^2} \le 1-\varepsilon\right\}. \tag{42}$$

To estimate the probability on the right-hand side of Eq. (42), we introduce three different events:

$$A(\eta') := \{|\|\vec{G}\|^2 - 1| < \eta'\}, \tag{43}$$

$$B(\eta'') := \left\{(1-\eta'')\frac{d_{eq}}{D} < \sum_{\beta=1}^{d_{eq}} |G_\beta|^2 < (1+\eta'')\frac{d_{eq}}{D}\right\}, \tag{44}$$

$$C(\eta''') := \left\{(1-\eta''')\frac{d_{eq}}{D} < \sum_{\beta=1}^{d_{eq}} \frac{|G_\beta|^2}{\|\vec{G}\|^2} < (1+\eta''')\frac{d_{eq}}{D}\right\}. \tag{45}$$

Let us now assume that

$$\frac{d_{eq}}{D} > 1 - \frac{\varepsilon}{2}. \tag{46}$$

We then have that

$$(1-\varepsilon/2)\frac{d_{eq}}{D} > 1 - \varepsilon + \frac{\varepsilon^2}{4} > 1-\varepsilon, \tag{47}$$

so that

$$C(\varepsilon/2) \subseteq \left\{(1-\varepsilon/2)\frac{d_{eq}}{D} < \sum_{\beta=1}^{d_{eq}} \frac{|G_\beta|^2}{\|\vec{G}\|^2}\right\}$$

$$\subseteq \left\{1-\varepsilon < \sum_{\beta=1}^{d_{eq}} \frac{|G_\beta|^2}{\|\vec{G}\|^2}\right\}, \tag{48}$$

and thus

$$p \ge 1 - D\mathbb{P}(C^c(\varepsilon/2)), \tag{49}$$

where the superscript c means complement. Our goal is to find a good upper bound for $\mathbb{P}(C^c(\varepsilon/2))$.

If the event $A(\eta')$ occurs for $0 < \eta' < \frac{1}{2}$ then

$$1-\eta' < \frac{1}{\|\vec{G}\|^2} < 1+2\eta', \tag{50}$$

and, consequently, if $A(\eta') \cap B(\eta'')$ occurs then

$$\frac{d_{eq}}{D}(1-\eta')(1-\eta'') < \frac{\sum_{\beta=1}^{d_{eq}} |G_\beta|^2}{\|\vec{G}\|^2} < \frac{d_{eq}}{D}(1+2\eta')(1+\eta''). \tag{51}$$

It is now easy to see that $A(\eta') \cap B(\eta'') \subseteq C(2\eta'+\eta''+2\eta'\eta'')$, so if we choose $\eta'=\eta''=\varepsilon/8$ we obtain that

$$A\left(\frac{\varepsilon}{8}\right) \cap B\left(\frac{\varepsilon}{8}\right) \subseteq C\left(\frac{3}{8}\varepsilon + \frac{1}{32}\varepsilon^2\right) \subseteq C(\varepsilon/2) \quad \text{for } 0<\varepsilon<1. \tag{52}$$

We thus have the following upper bound:

$$\mathbb{P}(C^c(\varepsilon/2)) \le \mathbb{P}(A^c(\varepsilon/8)) + \mathbb{P}(B^c(\varepsilon/8)). \tag{53}$$

To find an estimate of $\mathbb{P}(A(\varepsilon/8))$ and $\mathbb{P}(B(\varepsilon/8))$ we use the *large deviations principle*. It is convenient to use a slightly stronger version of this principle than usual (see Sec. 2.2.1 of [14]), which states that for a sequence of N independent and identically distributed (i.i.d.) random variables X_i,

$$\mathbb{P}\left(\left|\sum_{i=1}^{N}\frac{X_i}{N} - \mathbb{E}(X_1)\right| > \delta\right) \le 2e^{-NI[\mathbb{E}(X_1)+\delta]}, \tag{54}$$

where $I(x)$ is the *rate function* [14] associated with the distribution of X_i, defined to be

$$I(x) = \sup_{\theta>0}(\theta x - \log \mathbb{E}e^{\theta X_i}). \tag{55}$$

In our case, where X_i will be the square of a standard normal random variable, the rate function is

$$I(x) = \tfrac{1}{2}(x-1-\log x) \quad \forall\, x>1, \tag{56}$$

as a simple calculation shows.

To estimate $\mathbb{P}(A(\varepsilon/8))$, set

$$N=2D, \quad X_\beta = 2D(\mathrm{Re}\ G_\beta)^2, \quad X_{D+\beta} = 2D(\mathrm{Im}\ G_\beta)^2 \quad \text{for } \beta = 1,\ldots,D. \tag{57}$$

Thus, for $i=1,\ldots,2D$, X_i are i.i.d. variables with mean $\mathbb{E}X_i = 2D\mathbb{E}(\mathrm{Re}\ G_i)^2 = 1$; we thus obtain

$$\mathbb{P}(A^c(\varepsilon/8)) = \mathbb{P}\{|\|\vec{G}\|^2 - 1| > \varepsilon/8\} \tag{58}$$

$$= \mathbb{P}\left\{\left|\sum_{\beta=1}^{D}|G_\beta|^2 - 1\right| > \varepsilon/8\right\} \tag{59}$$

$$= \mathbb{P}\left\{\left|\sum_{i=1}^{2D}\frac{X_i}{2D} - 1\right| > \varepsilon/8\right\} \tag{60}$$

$$\le 2e^{-2DI(1+\varepsilon/8)} \tag{61}$$

$$= 2e^{-D[\varepsilon/8-\log(1+\varepsilon/8)]} \tag{62}$$

$$\le 2\exp\left(-\frac{D\varepsilon^2}{192}\right). \tag{63}$$

In the last step we have used $\log(1+x) \le x - x^2/3$ for $0<x<1/2$.

We use a completely analogous argument for B, setting

$$N=2d_{eq}, \quad X_\beta = 2D(\mathrm{Re}\ G_\beta)^2,$$

$$X_{D+\beta} = 2D(\mathrm{Im}\ G_\beta)^2, \quad \text{for } \beta = 1,\ldots,d_{eq}, \tag{64}$$

and obtain that

$$\mathbb{P}(B^c(\varepsilon/8)) = \mathbb{P}\left\{\left|\sum_{\beta=1}^{d_{eq}}|G_\beta|^2 - \frac{d_{eq}}{D}\right| / \frac{d_{eq}}{D} > \varepsilon/8\right\} \tag{65}$$

$$= \mathbb{P}\left\{\left|\sum_{i=1}^{2d_{eq}}\frac{X_i}{2d_{eq}} - 1\right| > \varepsilon/8\right\} \tag{66}$$

$$\le 2\exp\left(-\frac{d_{eq}\varepsilon^2}{192}\right). \tag{67}$$

From Eqs. (53), (63), and (67) it follows that

$$\mathbb{P}(C^c(\varepsilon/2)) \le 2\exp\left(-\frac{d_{eq}\varepsilon^2}{192}\right) + 2\exp\left(-\frac{D\varepsilon^2}{192}\right) \le 4\exp\left(-\frac{D\varepsilon^2}{384}\right), \tag{68}$$

where we have used $d_{eq} > D/2$. Therefore, by Eq. (49),

$$p \ge 1 - 4D\exp\left(-\frac{D\varepsilon^2}{384}\right). \tag{69}$$

The last term converges to zero as $D\to\infty$, so there exists $D_0>0$ such that for all $D>D_0$,

$$p \ge 1-\delta, \tag{70}$$

which is what we wanted to show. In order to check this for D_0 specified in Eq. (33) right after Lemma 1, note that the desired relation

$$4D\exp\left(-\frac{D\varepsilon^2}{384}\right) \le \delta \tag{71}$$

is equivalent to

$$D\left(\frac{\varepsilon^2}{384} - \frac{\log D}{D}\right) \ge \log(4/\delta). \tag{72}$$

Thus, it suffices that $D > 10^3\varepsilon^{-2}\log(4/\delta)$ and

$$\frac{\log D}{D} < 10^{-3}\varepsilon^2. \tag{73}$$

Since $\log D < \sqrt{D}$ for all positive numbers D, condition (73) will be satisfied if $\sqrt{D} > 10^3\varepsilon^{-2}$, i.e., if $D > 10^6\varepsilon^{-4}$. ■

IV. EXAMPLES OF SYSTEMS THAT DO NOT APPROACH THERMAL EQUILIBRIUM

We shall now present examples of atypical behavior, namely, examples of bad Hamiltonians, i.e., Hamiltonians for

which not all wave functions approach thermal equilibrium [or, equivalently, for which Eq. (24) is not satisfied]. According to Theorem 1, bad Hamiltonians form a very small subset of the set of all Hamiltonians. Of course, to establish that Eq. (24) holds for a particular Hamiltonian can be a formidable challenge. Moreover, the small subset might include all standard many-body Hamiltonians (e.g., all those which are a sum of kinetic and potential energies). But there is no *a priori* reason to believe that this should be the case.

The first example consists of two noninteracting subsystems. This can be expressed in the framework provided by example 1 in Sec. I B with the Hamiltonian $H=H_1+H_2+\lambda V$ by setting $\lambda=0$. Let $\{\phi_i^1\}$ be an orthonormal basis of $\mathcal{H}_1$ consisting of eigenvectors of H_1 with eigenvalues E_i^1, and let $\{\phi_j^2\}$ be one of $\mathcal{H}_2$ consisting of eigenvectors of H_2 with eigenvalues E_j^2. Clearly, for $\lambda=0$ not every wave function will approach thermal equilibrium. After all, in this case, $\phi_i^1 \otimes \phi_j^2$ forms an eigenbasis of H, while

$$\mathcal{H} = \mathrm{span}\{\phi_i^1 \otimes \phi_j^2 : E_i^1 + E_j^2 \in [E, E+\delta E]\}, \tag{74}$$

$$\mathcal{H}_{eq} = \mathrm{span}\{\phi_i^1 \otimes \phi_j^2 : E_i^1 \in [0.49E, 0.51E), \quad E_i^1 + E_j^2 \in [E, E+\delta E]\}. \tag{75}$$

Thus, any $\phi_i^1 \otimes \phi_j^2$ such that $E_i^1+E_j^2 \in [E, E+\delta E]$ but, say, $E_i^1 < 0.49E$, will be an example of an element of $\mathcal{H}$ that is orthogonal to $\mathcal{H}_{eq}$ and, as it is an eigenfunction of H, forever remains orthogonal to $\mathcal{H}_{eq}$.

As another example, we conjecture that some wave functions will fail to approach thermal equilibrium also when λ is nonzero but sufficiently small. We prove this now for a slightly simplified setting, corresponding to the following modification of example 1 of Sec. I B. For the usual energy interval $[E, E+\delta E]$, let $\mathcal{H}$ be, independently of λ, given by Eq. (74); and, instead of $H_1+H_2+\lambda V$, let H be given by

$$H = H(\lambda) = P(H_1 + H_2 + \lambda V)P, \tag{76}$$

where P is the projection to $\mathcal{H}$. Then H defines a time evolution on $\mathcal{H}$ that depends on λ. (Note that $\mathcal{H}$ is still an "energy shell" for all sufficiently small λ, as all nonzero eigenvalues of $H(\lambda)$ are still contained in an interval just slightly larger than $[E, E+\delta E]$, and the corresponding eigenvectors lie in $\mathcal{H}$.) Let $\mathcal{H}_{eq}$ for $\lambda \neq 0$ also be given by Eq. (75). Again, choose one particular ϕ_i^1 and one particular ϕ_j^2 (independently of λ), so that $E_i^1+E_j^2 \in [E, E+\delta E]$ and $E_i^1 < 0.49E$, and consider as the initial state of the system again

$$\psi(t=0) = \phi_i^1 \otimes \phi_j^2, \tag{77}$$

which evolves to

$$\psi(\lambda, t) = e^{-iH(\lambda)t} \phi_i^1 \otimes \phi_j^2. \tag{78}$$

Suppose for simplicity that $H(\lambda=0)=H_1+H_2$ is nondegenerate.[4] Then, according to standard results of perturbation theory [15], also $H(\lambda)$, regarded as an operator on $\mathcal{H}$, is nondegenerate for all $\lambda \in (-\lambda_0, \lambda_0)$ for some $\lambda_0 > 0$; moreover, its eigenvalues $E(\lambda)$ depend continuously (even analytically) on λ, and so do the eigenspaces. In particular, it is possible to choose for every $\lambda \in (-\lambda_0, \lambda_0)$ a normalized eigenstate $\phi(\lambda) \in \mathcal{H}$ of $H(\lambda)$ with eigenvalue $E(\lambda)$ in such a way that $\phi(\lambda)$ and $E(\lambda)$ depend continuously on λ, and $\phi(\lambda=0) = \phi_i^1 \otimes \phi_j^2$.

We are now ready to show that, for sufficiently small $\lambda > 0$,

$$\langle \psi(\lambda, t) | P_{eq} | \psi(\lambda, t) \rangle \approx 0 \tag{79}$$

for all t; that is, $\psi(\lambda, t)$ is nearly orthogonal to $\mathcal{H}_{eq}$ for all t, and thus is never in thermal equilibrium. To see this, note first that since $\phi(0) \approx \phi(\lambda)$ for sufficiently small λ, and since $e^{-iH(\lambda)t}$ is unitary, also

$$e^{-iH(\lambda)t} \phi(0) \approx e^{-iH(\lambda)t} \phi(\lambda) \tag{80}$$

(with error independent of t). Since the right-hand side equals

$$e^{-iE(\lambda)t} \phi(\lambda) \approx e^{-iE(\lambda)t} \phi(0), \tag{81}$$

we have that

$$\langle e^{-iH(\lambda)t} \phi(0) | P_{eq} | e^{-iH(\lambda)t} \phi(0) \rangle \approx \langle \phi(0) | P_{eq} | \phi(0) \rangle = 0. \tag{82}$$

This proves Eq. (79) with an error bound independent of t that tends to zero as $\lambda \to 0$.

Another example of bad Hamiltonians is provided by the phenomenon of *Anderson localization* (see in particular [16,17]): certain physically relevant Hamiltonians possess some eigenfunctions ϕ_α that have a spatial energy density function that is macroscopically nonuniform whereas wave functions in $\mathcal{H}_{eq}$ should have macroscopically uniform energy density over the entire available volume. Thus, some eigenfunctions are not close to $\mathcal{H}_{eq}$, violating Eq. (24).

V. COMPARISON WITH CLASSICAL MECHANICS

In classical mechanics, one would expect as well that a macroscopic system spends most of the time in the long run in thermal equilibrium. Let us define what thermal equilibrium means in classical mechanics. [We defined it for quantum systems in Eq. (8).] We denote a point in phase space by $X=(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$. Instead of the orthogonal decomposition of $\mathcal{H}$ into subspaces $\mathcal{H}_\nu$ we consider a partition of an energy shell Γ in phase space, $\Gamma = \{X : E \leq H(X) \leq E+\delta E\}$, into regions Γ_ν corresponding to different macrostates ν, i.e., if the microstate X of the system is in Γ_ν then the macrostate

[4] Since this requires that no eigenvalue difference of H_1, $E_i^1 - E_{i'}^1$, coincides with an eigenvalue difference of H_2, $E_j^2 - E_{j'}^2$, we need to relax our earlier assumption that systems 1 and 2 be identical; so, let them be almost identical, with slightly different eigenvalues, and let H_1 and H_2 each be nondegenerate.

of the system is ν. It has been shown [18] for realistic systems with large N that one of the regions Γ_ν, corresponding to the macrostate of thermal equilibrium and denoted Γ_{eq}, is such that, in terms of the (uniform or Liouville) phase-space volume measure μ on Γ,

$$\frac{\mu(\Gamma_{eq})}{\mu(\Gamma)} \approx 1. \tag{83}$$

Although the subspaces $\mathcal{H}_\nu$ play a role roughly analogous to the regions Γ_ν, a basic difference between the classical and the quantum cases is that while every classical phase point in Γ belongs to one and only one Γ_ν, and thus is in one macrostate, a quantum state ψ need not lie in any one $\mathcal{H}_\nu$, but can be a nontrivial superposition of vectors in different macrostates. (Indeed, almost all ψ do not lie in any one $\mathcal{H}_\nu$. That is why we defined being in thermal equilibrium in terms of ψ lying in a neighborhood of $\mathcal{H}_{eq}$, rather than lying in $\mathcal{H}_{eq}$ itself.)

The time evolution of the microstate X is given by the solution of the Hamiltonian equations of motion, which sends X (at time zero) to X_t (at time t), $t \in \mathbb{R}$. We expect that for realistic systems with a sufficiently large number N of constituents and for every macrostate ν, most initial phase points $X \in \Gamma_\nu$ will be such that X_t spends most of the time in the set Γ_{eq}. This statement follows if the system is ergodic,[5] but in fact is much weaker than ergodicity. Theorem 1 is parallel to this statement in that it implies, for typical Hamiltonians, that initial states [here, $\psi(0)$] out of thermal equilibrium will spend most of the time in thermal equilibrium; it is different in that it applies, for typical Hamiltonians, to *all*—rather than most—initial states $\psi(0)$.

VI. COMPARISON WITH THE LITERATURE

von Neumann [2] proved, as his "quantum ergodic theorem," a precise version of normal typicality (defined in Sec. II B); his proof requires much more effort, and more refined methods, than our proof of Theorem 1. However, his theorem assumes that the dimension d_ν of each macrospace $\mathcal{H}_\nu$ is much smaller than the full dimension D, and thus does not apply to the situation considered in this paper, in which one of the macrospaces, $\mathcal{H}_{eq}$, has the majority of dimensions. The reason von Neumann treated the more difficult case of small d_ν but left out the easier and particularly interesting case of the thermal equilibrium macrostate is that he had in mind a notion of thermal equilibrium different from ours. He thought of a thermal equilibrium wave function ψ, not as one in (or close to) a particular $\mathcal{H}_\nu$, but as one with $\|P_\nu\psi\|^2 \approx d_\nu/D$ for every ν, i.e., one for which $|\psi\rangle\langle\psi| \approx \rho_{mc}$ in a suitable coarse-grained sense. Because of this different focus, he did not consider the situation presented here. We also note that von Neumann's quantum ergodic theorem makes an assumption on H that we do not need in our Theorem 1; this assumption, known as a "no resonances" [8,10] or "nondegenerate energy gaps" [4] condition, asserts that

$$E_\alpha - E_\beta \neq E_{\alpha'} - E_{\beta'} \quad \text{unless} \begin{cases} \text{either } \alpha = \alpha', \ \beta = \beta' \\ \text{or } \alpha = \beta, \ \alpha' = \beta'. \end{cases} \tag{84}$$

The Schnirelman theorem [19] states that, in the semiclassical limit and under suitable hypotheses, the Wigner distribution corresponding to an eigenstate ϕ_α becomes the microcanonical measure. That is, ϕ_α has a property resembling thermal equilibrium, similar to our condition (24) expressing that all eigenstates are in thermal equilibrium. Srednicki [7] observed other thermal equilibrium properties in energy eigenstates of example systems, a phenomenon he referred to as "eigenstate thermalization."

The results of [4,5,8] also concern conditions under which a quantum system will spend most of the time in thermal equilibrium. For the sake of comparison, their results, as well as ours, can be described in a unified way as follows. Let us say that a system with initial wave function $\psi(0)$ *equilibrates* relative to a class $\mathcal{A}$ of observables if for most times τ,

$$\langle\psi(\tau)|A|\psi(\tau)\rangle \approx \mathrm{Tr}(\overline{|\psi(t)\rangle\langle\psi(t)|}A) \quad \text{for all } A \in \mathcal{A}. \tag{85}$$

We then say that the system *thermalizes* relative to $\mathcal{A}$ if it equilibrates and, moreover,

$$\mathrm{Tr}(\overline{|\psi(t)\rangle\langle\psi(t)|}A) \approx \mathrm{Tr}(\rho_{mc}A) \quad \text{for all } A \in \mathcal{A}, \tag{86}$$

with ρ_{mc} the microcanonical density matrix (in our notation, $1/D$ times the projection P to $\mathcal{H}$). With these definitions, the results of [4,5,8] can be formulated by saying that, under suitable hypotheses on H and $\psi(0)$ and for large enough D, a system will equilibrate, or even thermalize, relative to a suitable class $\mathcal{A}$.

Our result is also of this form. We have just one operator in $\mathcal{A}$, namely P_{eq}. We establish thermalization for arbitrary $\psi(0)$ assuming that H is nondegenerate and satisfies $\langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle \approx 1$ for all α, which (as we show) is typically true.

von Neumann's quantum ergodic theorem [2] establishes thermalization for a family $\mathcal{A}$ of commuting observables; $\mathcal{A}$ is the algebra generated by $\{M_1, \ldots, M_k\}$ in the notation of Sec. I A. He assumed that the dimensions of the joint eigenspaces $\mathcal{H}_\nu$ are not too small and not too large and that H obeys Eq. (84), he made an assumption about the relation between H and the subspaces $\mathcal{H}_\nu$ that he showed is typically true, and he admitted arbitrary $\psi(0)$. See [1] for further discussion. Rigol *et al.* [6] numerically simulated an example system and concluded that it thermalizes relative to a certain class $\mathcal{A}$ consisting of commuting observables.

Tasaki [8] as well as Linden *et al.* [4] considered a system coupled to a heat bath, $\mathcal{H}_{\text{total}} = \mathcal{H}_{\text{sys}} \otimes \mathcal{H}_{\text{bath}}$, and took $\mathcal{A}$ to contain all operators of the form $A_{\text{sys}} \otimes 1_{\text{bath}}$. Tasaki considered a rather special class of Hamiltonians and established thermalization assuming that

[5] A classical system is ergodic if and only if the time evolved microstate X_t spends, in the long run, a fraction of time in each (measurable) set $B \subseteq \Gamma$ that is equal to $\mu(B)/\mu(\Gamma)$ for μ-almost all X.

$$\max_{\alpha} |\langle \phi_\alpha | \psi(0) \rangle|^2 \ll 1, \tag{87}$$

a condition that implies that many eigenstates of H contribute to $\psi(0)$ appreciably and that can (more or less) equivalently be rewritten as

$$\sum_{\alpha} |\langle \phi_\alpha | \psi(0) \rangle|^4 \ll 1. \tag{88}$$

Under assumption (88) on $\psi(0)$, Linden *et al.* established equilibration for H satisfying Eq. (84). They also established a result in the direction of thermalization under the additional hypothesis that the dimension of the energy shell of the bath is much greater than $\dim \mathcal{H}_{\mathrm{sys}}$.

Reimann's mathematical result [5] can be described in the above scheme as follows. Let $\mathcal{A}$ be the set of all observables A with (possibly degenerate) eigenvalues between 0 and 1 such that the absolute difference between any two eigenvalues is at least (say) 10^{-1000}. He established equilibration for H satisfying Eq. (84), assuming that $\psi(0)$ satisfies Eq. (88).

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