On the Approach to Thermal Equilibrium of Macroscopic Quantum Systems

Sheldon Goldstein[*] and Roderich Tumulka,[†]

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Abstract

In joint work with J. L. Lebowitz, C. Mastrodonato, and N. Zanghì [2, 3, 4], we considered an isolated, macroscopic quantum system. Let $\mathscr{H}$ be a micro-canonical "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 macro-state at energy E corresponds to a subspace $\mathscr{H}_{eq}$ of $\mathscr{H}$ such that $\dim \mathscr{H}_{eq}/\dim \mathscr{H}$ is close to 1. We say that a system with state vector $\psi \in \mathscr{H}$ is in thermal equilibrium if ψ is "close" to $\mathscr{H}_{eq}$. We argue that for "typical" Hamiltonians, all initial state vectors ψ_0 evolve in such a way that ψ_t is in thermal equilibrium for most times t. This is closely related to von Neumann's quantum ergodic theorem of 1929.

1 Informal Statement of Result

The result we wish to describe concerns a macroscopic quantum system, described by a wave function ψ evolving according to a Schrödinger dynamics ($\hbar = 1$):

$$i\frac{\partial \psi_t}{\partial t} = H\psi_t \,. \tag{1}$$

Here is the statement:

[*]Departments of Mathematics and Physics, Rutgers University, Hill Center, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA. E-mail: oldstein@math.rutgers.edu

[†]Department of Mathematics, Rutgers University, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA. E-mail: tumulka@math.rutgers.edu

For *every* initial state ψ_0 of a *typical* macroscopic quantum system (e.g., a gas in a box), the system will spend *most* of its time in *thermal equilibrium*.

We will need to explain what we mean by "typical" and "most," though you can probably guess. But first we must explain what we mean by "thermal equilibrium."

2   What is Thermal Equilibrium?

There are, in fact, two basic views about what is meant by thermal equilibrium, corresponding to two different attitudes towards the foundations of statistical mechanics: the *individualist* view and the *ensemblist* view. According to the individualist *a system is in thermal equilibrium if it is in an appropriate pure state (given by a wave function or point in phase space).* According to the ensemblist *a system is in thermal equilibrium if it is in an appropriate statistical state (given by a density matrix or probability measure on phase space).* And depending upon what is intended by "appropriate" one obtains different individualist and ensemblist possibilities.

2.1   Individualist Equilibrium

In more detail, let's consider the meaning of equilibrium for an individualist for a classical macroscopic system. The state of the system is given by a point $X = (\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$ in its phase space, a point corresponding to the positions and velocities of its particles. The relevant part of the phase space is the energy surface $\Gamma = \{X : H(X) = E\}$, consisting of all phase points for which the energy H is the same value E. Then, depending on a choice of macro-variables, one may partition Γ into macro-states Γ_ν corresponding to different (small ranges of) values of the macro-variables, $\Gamma = \bigcup_\nu \Gamma_\nu$.

Here are two sketches of the partition into macro-states:

2
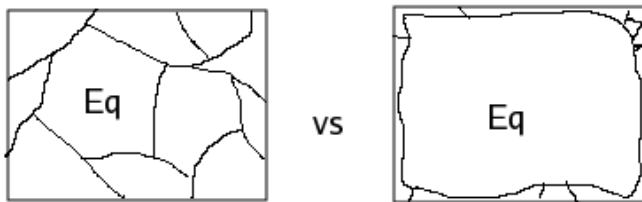
A crucial point is that the sketch on the left gives a completely distorted impression of the relative sizes of the macro-states. In particular, there will normally be one dominant macro-state, the equilibrium macro-state Γ_{eq}, that occupies almost the entire energy surface:

$$\frac{|\Gamma_{eq}|}{|\Gamma|} \approx 1$$

(using $|\cdot|$ for volume or area on the energy surface). With this is mind, we say that *a system is in equilibrium if its phase point is in the equilibrium macro-state, $X \in \Gamma_{eq}$.*

For a macroscopic quantum system the state of the system is given by its (normalized) wave function $\psi = \psi(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_N)$ ($\|\psi\| = 1$). We shall assume that this belongs to the energy shell $\mathscr{H} = \mathrm{span}\{\phi_\alpha : E_\alpha \in [E, E + \delta E]\}$, spanned by the energy eigenstates ϕ_α whose eigenvalues E_α belong to the indicated range, i.e., $\psi = \sum_\alpha c_\alpha \phi_\alpha$, $H\phi_\alpha = E_\alpha \phi_\alpha$. Then, instead of a partition into macro-states, we have an orthogonal decomposition into macro-spaces $\mathscr{H}_\nu$, corresponding more or less to different (small ranges of) values of the macro-variables (suitably "rounded" so that they commute),

$$\mathscr{H} = \bigoplus_\nu \mathscr{H}_\nu. \tag{2}$$

We assume that there is one dominant macro-space $\mathscr{H}_{eq}$:

$$\frac{\dim \mathscr{H}_{eq}}{\dim \mathscr{H}} \approx 1.$$

We say that *the system is in equilibrium if its wave function ψ is near $\mathscr{H}_{eq}$,* meaning that the projection $P_{eq}\psi$ of ψ into $\mathscr{H}_{eq}$ is almost all of ψ, i.e., that

$$\langle \psi | P_{eq} | \psi \rangle \approx 1. \tag{3}$$

2.2   Ensemblist Equilibrium

For an ensemblist a system is in equilibrium if its state X is random, or its quantum state is a mixture, with distribution or density matrix

$$\rho = \rho_{mc} \quad \text{or} \quad \rho = \rho_{can} = e^{-\beta H}/Z,$$

where ρ_{mc} describes the microcanonical ensemble. This formulation has the defect that an individual system can't be in equilibrium and the virtue of being precise. It also has the virtue that it admits of a clean simple notion of approach to equilibrium.

2.3 Approach to Thermal Equilibrium

For an ensemblist a system approaches equilibrium of its time-evolving statistical state ρ_t has the obvious long-time limit:

$$\rho_t \longrightarrow \rho_{mc} \text{ (or } \rho_{can}\text{) as } t \to \infty$$

in a suitable sense. This sort of *mixing* behavior, though rare and hard to prove for realistic deterministic dynamical systems, is a genuine mathematical possibility.

As a natural first attempt at an individualist formulation of approach to equilibrium, consider the condition that $X_t \in \Gamma_{eq}$ (or near Γ_{eq}) as $t \to \infty$, i.e., that $\langle \psi_t | P_{eq} | \psi_t \rangle \approx 1$ for $t \to \infty$. This is typically impossible, because of the phenomenon of Poincaré recurrence. It will typically not be the case that the system is in, or near, equilibrium for all sufficiently large times. Rather what is meant by *approach to equilibrium* for an individualist, and what we mean by it here, is that $X_t \in \Gamma_{eq}$ or, in the quantum case, with which we are concerned here,

$$\langle \psi_t | P_{eq} | \psi_t \rangle \approx 1$$

for *most* (sufficiently large) t (even when the system is initially not in equilibrium).

2.4 Equilibrium is Typical

It is important to recognize that with this (equation (3)) understanding of equilibrium, for *most* $\psi \in \mathscr{H}$ the system is indeed in equilibrium—just as in the classical case. Here the sense of "most" is given by the microcanonical distribution $\mu_{mc} = \mu$ on $\mathscr{H}$, i.e., the uniform distribution over the unit sphere in $\mathscr{H}$:

$$\langle \psi | P_{eq} | \psi \rangle \approx 1 \text{ for } \mu\text{-most } \psi s .$$

This is easily seen by computing the microcanonical average

$$
\begin{aligned}
\int \mu(d\psi) \langle \psi | P_{eq} | \psi \rangle &= \text{Tr} \left[\left(\int \mu(d\psi) | \psi \rangle \langle \psi | \right) P_{eq} \right] \\
&= \text{Tr} \left[\rho_{mc} P_{eq} \right] = \frac{\dim \mathscr{H}_{eq}}{\dim \mathscr{H}} \approx 1 ,
\end{aligned}
$$

where $\rho_{mc} = I / \dim \mathscr{H}$ (and $\mathrm{Tr} P_{eq} = \dim \mathscr{H}_{eq}$). Since $\langle \psi | P_{eq} | \psi \rangle$ can be no greater than 1, it follows that it must be near 1 for μ-most ψs.

That equilibrium is in this sense typical is crucial to the individualist understanding of the notion. However, it does have the consequence that the initial wave functions ψ_0 with which we are concerned for the issue of approach to equilibrium are atypical. We would like it to be the case that even for "most" non-equilibrium initial wave functions we have approach to equilibrium. The best that we could hope for in this regard is that we have approach to equilibrium for all such wave functions.

3 Absolute Thermalization and Eigenstate Thermalization

When a system is such that we have approach to equilibrium for *all* initial wave functions ψ_0, we say that we have *absolute thermalization* (AT). Clearly, a necessary condition for AT is that

$$\langle \phi_\alpha | P_{eq} | \phi_\alpha \rangle \approx 1 \text{ for all } \alpha, \tag{4}$$

since the energy eigenstates ϕ_α, possible initial states, are stationary states. Equation (4) is a version of what Srednicki [8] has called *eigenstate thermalization* (ET).

It is also sufficient, as is easily seen by computing the time-average of $\langle \psi_t | P_{eq} | \psi_t \rangle$. Writing $\overline{f(t)}$ for the time average of f,

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

we have that

$$\overline{\langle \psi_t | P_{eq} | \psi_t \rangle} = \mathrm{Tr} \left[\overline{|\psi_t\rangle\langle\psi_t|} P_{eq} \right] \,. \tag{5}$$

With

$$\psi_0 = \sum_{\alpha=1}^{D} c_\alpha |\phi_\alpha\rangle \quad (D = \dim \mathscr{H})$$

and hence

$$\psi_t = \sum_{\alpha=1}^{D} e^{-iE_\alpha t} c_\alpha |\phi_\alpha\rangle$$

we thus have that

$$\overline{|\psi_t\rangle\langle\psi_t|} = \sum_{\alpha,\beta} \underbrace{\overline{e^{-i(E_\alpha - E_\beta)t}}}_{\delta_{\alpha\beta}} c_\alpha c_\beta^* |\phi_\alpha\rangle\langle\phi_\beta| = \sum_\alpha |c_\alpha|^2 |\phi_\alpha\rangle\langle\phi_\alpha|\,.$$

Inserting this into (5), we find that

$$\overline{\langle\psi_t|P_{eq}|\psi_t\rangle} = \sum_\alpha |c_\alpha|^2 \langle\phi_\alpha|P_{eq}|\phi_\alpha\rangle\,. \tag{6}$$

Since $\langle\psi_t|P_{eq}|\psi_t\rangle$ can't be greater that 1, it follows from (6) and (4) that it must be near 1 for most times. Hence ET is indeed a sufficient condition for AT,

$$\mathrm{ET} \Rightarrow \mathrm{AT}\,.$$

3.1 Eigenstate Thermalization

Even though equilibrium is typical, since ET requires that *all* energy eigenstates in the microcanonical subspace $\mathscr{H}$, of which there are a great many, be in equilibrium, you might imagine that ET is a rather stringent condition. It can be shown [2], however, that ET in facts holds for a typical Hamiltonian H.

The meaning here of "typical" is in the sense of most Hs as provided by the uniform distribution on orthonormal bases of $\mathscr{H}$: Fix the energies $E_1,\dots,E_D$ (assumed nondegenerate). Let

$$H = \sum_\alpha E_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$$

with the orthonormal basis $\phi_\alpha, \alpha = 1,\dots D$, uniformly distributed. Equivalently, let

$$H = UH_0U^*, \quad H_0 = \sum_\alpha E_\alpha |\chi_\alpha\rangle\langle\chi_\alpha|$$

with χ_α any orthonormal basis of $\mathscr{H}$ and U a uniformly (Haar) distributed unitary on $\mathscr{H}$. By a typical Hamiltonian we refer to the distribution of such a random Hamiltonian H.

To appreciate why ET might be expected to hold for a typical Hamiltonian H, choose the basis $\{\chi_\alpha\}$ in such a way that the first $d_{eq} = \dim\mathscr{H}$ basis

vectors lie in $\mathcal{H}_{eq}$. Then

$$\langle \phi_\alpha | P_{eq} | \phi_\alpha \rangle = \sum_{\beta=1}^{d_{eq}} |U_{\beta\alpha}|^2 \tag{7}$$

with

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

where $U_{\beta\alpha}$ is uniformly distributed unitary $D \times D$ matrix. The distribution of (7) is independent of α, and the crucial estimate is that of the probability p that $\sum_{\beta=1}^{d_{eq}} |U_{\beta\alpha}|^2$ fails to be near 1.

For fixed α the $U_{\beta\alpha}$s are approximately independent complex Gaussian random variables with mean 0 and variance $1/D$. Suitably using large deviations estimates for independent Gaussians, p can be shown to be sufficiently small.

4   Precise Statement of Result

For the record, here is a precise statement of the main result:

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; 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 in the sense that

$$\liminf_{T \to \infty} \frac{1}{T} \left| \left\{ 0 < t < T : \langle \psi_t | P_{eq} | \psi_t \rangle > 1 - \eta \right\} \right| \geq 1 - \delta', \tag{8}$$

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

We don't want to go into many details here. But we do want to note that $\delta \; (\approx 0)$ makes precise what we have meant by most Hs, $\delta' \; (\approx 0)$ most times, and $\eta \; (\approx 0)$ how near $\langle \psi_t | P_{eq} | \psi_t \rangle$ must be to 1.

5 Von Neumann's Quantum Ergodic Theorem (1929) [10]

Here is an informal statement of von Neumann's quantum ergodic theorem:

> For *every* initial state ψ_0 of a *typical* macroscopic quantum system, the system will spend *most* of its time in *thermal equilibrium.*

This should seem rather similar to the earlier informal statement of the result I've been discussing up to this point. And, as a matter of fact, "every" and "most" mean here exactly what they meant there, and "typical" means almost the same thing. But the meaning here of "thermal equilibrium" is rather different.

In the orthogonal decomposition (2) of $\mathscr{H}$ into macro-spaces $\mathscr{H}_\nu$, let $d_\nu = \dim \mathscr{H}_\nu$ and let P_ν be the corresponding projections. For von Neumann a system with wave function ψ is in thermal equilibrium if, instead of (3), we have that

$$\langle\psi|P_\nu|\psi\rangle \approx d_\nu/D \tag{9}$$

for all ν. And as a sufficient condition for absolute thermalization AT+ for this more stringent notion of equilibrium, von Neumann provides a strengthening ET++ of ET. ET++ is in fact a strengthening of a condition ET+, namely that for all ν

$$\langle\phi_\alpha|P_\nu|\phi_\alpha\rangle \approx d_\nu/D \tag{10}$$

for all α, itself a strengthening of ET naturally suggested by comparing (3) and (9).

To better appreciate the significance of (9), observe that

$$\int \mu(d\psi)\langle\psi|P_\nu|\psi\rangle = \text{Tr}\left[\rho_{mc}P_\nu\right] = d_\nu/D\,.$$

In particular, (9) is the same thing as

$$\langle\psi|P_\nu|\psi\rangle \approx \text{Tr}\left[\rho_{mc}P_\nu\right]\,,$$

i.e., the requirement that the quantum averages of the macro-projections P_ν agree with their micro-canonical averages.

ET++ involves a certain non-resonance condition [10] (requiring non-degenerate energy gaps) together with the following:

$$\max_{\alpha\neq\beta}\left|\langle\phi_\alpha|P_\nu|\phi_\beta\rangle\right|^2 + \max_\alpha\left(\langle\phi_\alpha|P_\nu|\phi_\alpha\rangle - \frac{d_\nu}{D}\right)^2 \ll 1\,. \tag{11}$$

The second term on the left hand side of (11) corresponds to ET+, which implies that

$$\overline{\langle\psi_t|P_\nu|\psi_t\rangle} \approx \frac{d_\nu}{D}$$

in the same way that ET implies AT. But ET+ does not imply AT+, because $\langle\psi_t|P_\nu|\psi_t\rangle$ could have significant fluctuations above and below its mean. The first term is needed to control these fluctuations, via bounds on

$$\overline{\left(\langle\psi_t|P_\nu|\psi_t\rangle - \frac{d_\nu}{D}\right)^2}.$$

Von Neumann showed that ET++ indeed implies AT+. He also showed that ET++ is satisfied for a typical Hamiltonian. To do the latter is considerably more difficult than showing this for ET. (Because of certain assumptions on the dimensions of macro-spaces needed by von Neumann, the result in Section (4) is not a consequence of the quantum ergodic theorem.)

5.1 A Remark on Varieties of Individualism (Quantum Case)

Von Neumann's quantum ergodic theorem has both individualist and ensemblist aspects. It is individualist in that the relevant notion of equilibrium is for an individual pure state; it is ensemblist in that what it demands of that pure state is that it resemble the microcanonical ensemble. We're inclined to say that the quantum ergodic theorem is quasi-individualist—individualist by accident or necessity—and not pure individualist. This is true also for many of the related results—in which the individualism permits the extraction of thermal statistics without having to make any detailed a priori probablistic assumptions—upon which we shall now touch.

6 Related Results

Versions of eigenstate thermalization have been discussed by Schnirelman, see [1], and by M. Srednicki [8]. Results on equilibration and thermalization have been obtained by N. Linden, S. Popescu, A.J. Short, and A. Winter [5], by P. Reimann [6], by H. Tasaki [9], and by M. Rigol, V. Dunjko, and M. Olshanii [7].

Most of the equilibration and thermalization results say something in the vicinity of the following: *For physical initial states ψ_0 of suitable macroscopic quantum systems, the system will spend most of its time in thermal equilibrium.* Different results may involve different notions of "physical" and of "suitable." Here we wish only to mention that the various "thermal equilibrium" conditions involved are of the form

$$\langle \psi | A | \psi \rangle \approx \mathrm{Tr}\left[\rho_{mc} A\right]$$

for all $A \in \mathscr{A}$, with the different choices of a class $\mathscr{A}$ of observables corresponding to different notions of thermal equilibrium. For example, for von Neumann $\mathscr{A}$ consists of macroscopic observables, and for Linden et al. of observables for a small subsystem of a larger system.

7   Remark on Typicality

We quote here from [3]:

> When employing the method of appeal to typicality, one usually uses the language of probability theory. But that does not imply that any of the objects considered is random in reality. Rather, it means that certain sets (of wave functions, of orthonormal bases, etc.) have certain sizes (e.g., close to 1) in terms of certain natural (normalized) measures of size. That is, one describes the behavior that is *typical* of wave functions, orthonormal bases, etc.. However, since the mathematics is equivalent to that of probability theory, it is convenient to adopt that language. For this reason, using a normalized measure μ does not mean making an "assumption of equal probability," even if one uses the word "probability." Rather, it means that, if a condition is true of most ..., or most H, this fact may suggest that the condition is also true of a concrete given system, unless we have reasons to expect otherwise.
>
> Of course, a theorem saying that a condition is true of the vast majority of systems does not *prove* anything about a concrete given system; if we want to know for sure whether a given system is normal for every initial wave function, we need to check the relevant condition .... Nevertheless, a typicality theorem is,

as we have suggested, illuminating; at the very least, it is certainly useful to know which behaviour is typical and which is exceptional. . . .

The method of appeal to typicality belongs to a long tradition in physics, which includes also Wigner's work on random matrices of the 1950s. In the words of Wigner . . . :

> One [. . .] deals with a specific system, with its proper (though in many cases unknown) Hamiltonian, yet pretends that one deals with a multitude of systems, all with their own Hamiltonians, and averages over the properties of these systems. Evidently, such a procedure can be meaningful only if it turns out that the properties in which one is interested are the same for the vast majority of the admissible Hamiltonians.

This method was used by Wigner to obtain specific new and surprising predictions about detailed properties of complex quantum systems in nuclear physics.

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