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Eigenstate thermalization: Deutsch's approach and beyond

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Abstract

The eigenstate thermalization hypothesis postulates that the energy eigenstates of an isolated many-body system are thermal, i.e., each of them already yields practically the same expectation values as the microcanonical ensemble at the same energy. Here, we review, compare, and extend some recent approaches to corroborate this hypothesis and discuss the implications for the system's equilibration and thermalization.

1. Introduction

The relaxation of a macroscopic many-body system towards thermal equilibrium is a very common phenomenon, but has still not been satisfactorily understood theoretically [1, 2]. In particular, isolated systems and their text book description at equilibrium by a microcanonical ensemble [3] have recently regained considerable attention [4–6]. An immediate first puzzle is the mere fact that the system apparently approaches a steady long time limit though the quantum mechanical time evolution of a non-equilibrium initial state is well-known *not* to become asymptotically time-independent (see e.g. section 2 below). As one possible way out, one could, for instance, try to show that after a sufficiently long 'equilibration time', the expectation values of pertinent observables become 'practically constant' (fluctuations remain below any reasonable resolution limit) for 'practically all' later times (exceptions do exists—e.g. due to quantum revivals—but are exceedingly rare). Indeed, results of this type have been established under fairly weak and plausible assumptions about the initial state, the Hamiltonian, and the observables of the considered system [2, 7–12]. As an natural next step, quantitative estimates of the above mentioned equilibration times are currently attracting increasing interest [10, 13–16]. This is a very important but also quite difficult issue in its own right, which goes beyond the scope of our present paper.

Here, we rather will focus on another natural next issue, named thermalization: given that the expectation value of an observable equilibrates in the above sense, how well does this long-time limit agree with the corresponding microcanonical expectation value, as predicted by equilibrium statistical mechanics? A sufficient condition for a good such agreement is the so-called eigenstate thermalization hypothesis (ETH), essentially postulating that the expectation values of pertinent observables exhibit negligible variations for all energy eigenstates with sufficiently close energy eigenvalues. This hypothesis has its roots in closely related conjectures by Berry and Voros about the energy eigenstates of (fully) chaotic systems in the semiclassical limit, see e.g. equation (9) in [17] and equation (6.17) in [18]. Their implications for the (diagonal as well as off-diagonal) matrix elements in energy representation for observables with a well-behaved classical limit were further explored by Feingold and coauthors [19–21]. The key role of ETH for thermalization in high dimensional chaotic systems in the semiclassical regime was first recognized by Srednicki[1] [22–24]. Even earlier, its actual validity was numerically (and implicitly) exemplified and adopted as an explanation for the observed thermalization in a spin-chain model by Jensen and Shankar [25]. More recently, the seminal paper by Rigol *et al* [26] introduced the term ETH, pinpointed its importance for thermalization, and stimulated numerous, predominantly numerical studies on the validity of ETH for a large variety of specific models (mostly spin-

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[1] It may be worth noting that in those semiclassical studies [17–24] the term 'microcanonical ensemble' is used quite differently than in the present paper (see section 3), namely referring to classical phase space averages over an *infinitely thin* energy surface.

chain- or Hubbard-like), initial conditions (often involving some quantum quench), and observables (mainly few-body or local), see e.g. [27–40].

Mathematically, the validity of ETH could be demonstrated so far only in special cases, namely for the eigenfunctions of the Laplace operator on an arbitrary dimensional compact Riemannian manifold whose geodesic flow is ergodic. If also the considered observables are sufficiently well-behaving, then ETH can be proven to hold for the vast majority of all eigenfunctions with asymptotically large eigenvalues [41–43].

Another analytical key work is due to Deutsch, implicitly verifying ETH for the vast majority of systems, whose Hamiltonians have been sampled according to a certain random matrix ensemble [44–46]. Here, we generalize this approach by Deutsch and unravel its close connection with other recent explorations of thermalization, especially by Goldstein and coworkers [5, 13, 16, 47–49].

2. Equilibration

We consider a large (macroscopic but finite), isolated system, modelled in terms of a Hamiltonian H with eigenvalues E_n and eigenvectors $|n\rangle$, where $n \in \mathbb{N}$ and $E_{n+1} \geqslant E_n$. System states—either pure or mixed—are described by density operators $\rho(t)$, evolving according to $\rho(t) = U_t \rho(0) U_t^\dagger$ with propagator $U_t := \exp\{-iHt\}$ and $\hbar = 1$. It follows that $\rho_{mn}(t) := \langle m| \rho(t) |n\rangle$ is given by $\rho_{mn}(0) \exp[-i(E_m - E_n)t]$, i.e., unless the system was already in a steady state initially, it remains time-dependent forever. In other words, non-equilibrium initial states do not seem to 'equilibrate' towards a steady long-time limit in an obvious way.

Observables are represented by self-adjoint operators A with expectation values $\text{Tr}\{\rho(t)A\}$. In order to model real experimental measurements it is, however, not necessary to admit any arbitrary self-adjoint operator [50–57]. Rather, it is sufficient to focus on experimentally realistic observables in the following sense [7, 58]: any observable A must represent an experimental device with a finite range of possible outcomes of a measurement,

$$\Delta_A := a_{\max} - a_{\min}, \tag{1}$$

where $a_{\max}$ and $a_{\min}$ are the largest and smallest eigenvalues of A. Moreover, this working range Δ_A of the device must be limited to experimentally reasonable values compared to its resolution limit δA. Indeed, real measurements usually yield at most 10–20 relevant digits, i.e. it is sufficient to consider range-to-resolution ratios $\Delta_A/\delta A \leqslant 10^{20}$.

Next we define for any given $\delta A > 0$ and $T > 0$ the quantity

$$T_{\delta A} := \left| \left\{ 0 \leqslant t \leqslant T : \left| \text{Tr}\{\rho(t)A\} - \text{Tr}\{\rho_{\text{eq}}A\} \right| \geqslant \delta A \right\} \right|, \tag{2}$$

where $|\{...\}|$ denotes the size (Lebesgue measure) of the set $\{...\}$ and where the time-independent, so-called equilibrium or diagonal ensemble ρ_{eq} is defined as the diagonal part of $\rho(0)$, i.e. $(\rho_{\text{eq}})_{mn} := \delta_{mn}\rho_{nn}(0)$. As detailed e.g. in [11, 12], one then can show that

$$\frac{T_{\delta A}}{T} \leqslant 2\left(\frac{\Delta_A}{\delta A}\right)^2 \max_n\{\rho_{nn}(0)\} \tag{3}$$

for all sufficiently large T. For the sake of simplicity, we also have taken here for granted that the energy gaps $E_m - E_n$ are finite and mutually different for all pairs $m \neq n$. Generalizations have been worked out e.g. in [9–12].

According to (2), the left-hand side of (3) represents the fraction of all times $t \in [0, T]$, for which there is an experimentally resolvable difference between the true expectation value $\text{Tr}\{\rho(t)A\}$ and the time-independent equilibrium expectation value $\text{Tr}\{\rho_{\text{eq}}A\}$. On the right-hand side, $\Delta_A/\delta A$ is the above mentioned range-to-resolution ratio and $\max_n\{\rho_{nn}(0)\}$ represents the largest occupation probability of an energy eigenstate (note that the $\rho_{nn}(t)$ are conserved quantities).

For a macroscopic N-body system there are roughly $10^{O(N)}$ energy eigenstates with eigenvalues in every interval of 1J beyond the ground state energy [3]. Since $N = O(10^{23})$, the energy levels are thus unimaginably dense and even the most careful experimentalist will not be able to populate only a few of them with significant probabilities $\rho_{nn}(0)$. In the generic case we thus expect [7, 58] that—even if the system's energy is fixed up to an extremely small experimental uncertainty, and even if the energy levels are populated extremely unequally—the largest population $\rho_{nn}(0)$ will still be extremely small (compared to $\sum_n \rho_{nn}(0) = 1$), overwhelming by far the factor $(\Delta_A/\delta A)^2$ on the right-hand side of (3).

Since the level populations $\rho_{nn}(0)$ are the result of the system preparation, a more detailed understanding and quantification of those terms necessarily requires the modelling of such a preparation procedure. We come back to this point in section 7, where arguments will be provided that

$$\max_n \left\{ \rho_{nn}(0) \right\} = 10^{-\mathrm{O}(N)} \tag{4}$$

can be expected in many cases.

From (3) together with (4) we can conclude that the system generically equilibrates in the sense that it behaves in every possible experimental measurement exactly as if it were in the equilibrium state ρ_{eq} for the overwhelming majority of times within any sufficiently large time interval $[0, T]$.

3. Thermalization

Next we address the question of whether, and to what extent, the above discussed equilibrium expectation value $\mathrm{Tr}\{\rho_{\mathrm{eq}}A\}$ is in agreement with the corresponding microcanonical expectation value, as predicted by the textbooks on equilibrium statistical mechanics for our isolated N-body system at hand [3].

To begin with, $I_{\mathrm{mic}} := [E - \Delta E, E]$ denotes the usual microcanonical energy window about the (approximately known and thus preset) system energy E, whose width ΔE is macroscopically small (below the experimental resolution limit) but microscopically large (much larger than the typical energy level spacing $E_{n+1} - E_n$). The number of energy eigenvalues E_n contained in I_{mic} is denoted as D and is typically very large. The corresponding microcanonical ensemble is given by

$$\rho_{\mathrm{mic}} := \frac{1}{D} \sum_{\mathrm{mic}} |n\rangle \langle n|, \tag{5}$$

where the sum $\sum_{\mathrm{mic}}$ runs over all n with $E_n \in I_{\mathrm{mic}}$. In other words, $\rho_{nn}^{\mathrm{mic}} = 1/D$ if $E_n \in I_{\mathrm{mic}}$ and $\rho_{nn}^{\mathrm{mic}} = 0$ otherwise. Hence, the expectation value of A in the microcanonical ensemble takes the form

$$\mathrm{Tr}\left\{\rho_{\mathrm{mic}}A\right\} = \sum_n \rho_{nn}^{\mathrm{mic}} A_{nn} = \frac{1}{D} \sum_{\mathrm{mic}} A_{nn}. \tag{6}$$

On the other hand, recalling that $(\rho_{\mathrm{eq}})_{mn} := \delta_{mn} \rho_{nn}(0)$ implies

$$\mathrm{Tr}\left\{\rho_{\mathrm{eq}}A\right\} = \sum_n \rho_{nn}(0) \, A_{nn}. \tag{7}$$

As usual, we henceforth assume that the system is experimentally prepared at the preset macroscopic energy E, i.e. also the $\rho_{nn}(0)$'s are negligibly small for energies E_n outside I_{mic}. However, within I_{mic} the actual populations $\rho_{nn}(0)$ are still largely unknown and cannot be controlled by the experimentalist. In general we therefore have to admit the possibility that they considerably vary in a largely unknown (pseudo-random) fashion even between neighbouring n's.

The problem of thermalization thus amounts to showing that the difference between (6) and (7) is negligible in spite of the lack of knowledge about the $\rho_{nn}(0)$'s.

4. Eigenstate thermalization hypothesis (ETH)

As mentioned in the introduction, the ETH consists in the surmise that the expectation values A_{nn} of an observable A hardly differ for eigenstates $|n\rangle$ of a many-body Hamiltonian H with sufficiently close energy eigenvalues E_n [22–24, 26, 44, 45]. In particular, if the variations of the A_{nn}'s are negligible over the entire microcanonical energy window I_{mic}, then the (approximate) equality of (6) and (7) follows immediately. In this sense, ETH is a sufficient (but not necessary) condition for thermalization.

Similarly as for the microcanonical ensemble in (6), ETH also implies the equivalence of ρ_{eq} in (7) with a large variety of other pure or mixed steady states, whose level populations are mainly concentrated within the energy window I_{mic}. On the one hand, this includes other equilibrium ensembles such as the canonical ensemble, provided the considered energy interval ΔE is large enough to accommodate all notably populated energy levels. (As we will see later, the latter requirement is in fact quite problematic.) On the other hand, even a single energy eigenstate $|n\rangle$ with $E_n \in I_{\mathrm{mic}}$ will do. In other words [26], such an energy eigenstate encapsulates all properties of the considered many-body system at thermal equilibrium!

Two rather delicate problems, which any 'validation' of ETH has to resolve, are as follows: (i) for any given Hamiltonian H, one can readily construct (*a posteriori*) observables A which violate ETH, e.g. $A_{nn} = (-1)^n$ and arbitrary A_{mn} for $m \neq n$. (In contrast to what [39] might suggest, an ETH-violating observable thus needs *not* be a conserved quantity.) In particular, this example implies that ETH cannot be satisfied simultaneously for all observables, and in fact not even for all experimentally realistic observables as specified below equation (1). (ii) While ETH claims that expectation values A_{nn} are (practically) equal for sufficiently close energy eigenvalues E_n, generically there are—of course—notable differences $A_{mm} - A_{nn}$ when $E_m - E_n$ is *not* small. But how can the

observable A 'feel' whether the two eigenstates $|m\rangle$ and $|n\rangle$ of H belong to similar energies or not, without any *a priori* knowledge about the Hamiltonian H?

At first glance, it thus might seem unavoidable to somehow restrict the set of admissible observables. Indeed, the early explorations of ETH [17–24] solely had in mind semiclassical (small $\hbar$) systems, which are classically chaotic, in conjunction with observables, which are $\hbar$-independent and derive from smooth classical phase space functions (see section 1). In contrast, the more recent, predominantly numerical studies were mainly focused on spin-chain- and Hubbard-like models [27–40] (i.e. without an obvious classical limit), and on few-body or local observables. Yet another option would be to only admit macroscopic observables, see section 8 below. In either case, it is still not obvious whether and why such a restricted class of observables may get around the above mentioned problems (i) and (ii). The solution of those problems within our present approach will be discussed in section 9.

5. The approach by Deutsch

In this section, we reconsider the approach by Deutsch, originally published in [44]. For the detailed calculations, announced as [6] therein, see [45]. For an updated summary, see also [46].

5.1. Random matrix model

Following Deutsch [44] we consider Hamiltonians H of the form

$$H = H_0 + V, \tag{8}$$

consisting of an 'unperturbed' part H_0 and a 'perturbation' V. As before, eigenvectors and eigenvalues of H are denoted as $|n\rangle$ and E_n with $E_{n+1} \geqslant E_n$. Likewise, those of H_0 are denoted as $|n\rangle_0$ and E_n^0 with $E_{n+1}^0 \geqslant E_n^0$.

Typical examples one has in mind [44] are H_0 which describe a non-interacting many-body system, e.g. an ideal gas in a box, while V accounts for the particle–particle interactions. Further examples are so-called quantum quenches: H_0 describes the system for times $t < 0$, while H applies to $t \geqslant 0$. In other words, some external condition or some system property suddenly changes at time $t = 0$.

In various such examples, the perturbation matrix

$$V_{mn}^0 := {}_0\langle m|\, V\, |n\rangle_0 \tag{9}$$

is often expected or numerically found to be a banded matrix [21, 44, 59, 60], i.e., the typical magnitude of V_{mn}^0 decreases with increasing $|m - n|$ towards zero. Furthermore, in the above mentioned example where H_0 describes a non-interacting many-body system, the perturbation matrix V_{mn}^0 is usually very sparse, i.e., only a small fraction of all matrix elements is non-zero [60–62].

In any case, the perturbation V is required to be sufficiently weak so that the two systems H and H_0 still exhibit similar thermodynamic properties at the considered system energy E, in particular similar densities of the energy levels, see above equation (4).

As a next step, the common lore of random matrix theory is adopted [44, 47, 61]: one samples matrices V_{mn}^0 from a certain random matrix ensemble with statistical properties which imitate reasonably well the main features of the 'true' perturbation V (band structure, sparsity etc), and it is assumed that if a certain property can be shown to apply to the overwhelming majority of such randomly sampled V-matrices, then it will also apply to the actual (non-random) V in (8). *A priori*, such a random matrix approach may appear 'unreasonable' since most of those randomly sampled perturbations V amount to systems which are physically very different from the one actually modelled in (8). Yet, in practice such a random matrix approach turned out to be surprisingly successful in a large variety of specific examples [61], and hence, as in Deutsch's work [44], will be tacitly taken for granted from now on.

5.2. General framework

The randomness of V entails via in (8) a randomization of the eigenstates $|n\rangle$ of H and hence of the basis-transformation matrix

$$U_{mn} := \langle m|n\rangle_0. \tag{10}$$

Likewise, any given observable A and its matrix elements in the unperturbed basis

$$A_{mn}^0 := {}_0\langle m|\, A\, |n\rangle_0 \tag{11}$$

are non-random quantities, while

$$A_{mn} := \langle m|\, A\, |n\rangle \tag{12}$$

will be the elements of a random matrix, inheriting the randomness of the U-matrix via

$$A_{mn} = \sum_{jk} U_{mj} A_{jk}^0 U_{nk}^{\star}. \tag{13}$$

Demonstrating ETH thus amounts to showing that $A_{mm} - A_{nn}$ is small for most V's and sufficiently close m and n. Formally, this will be achieved by considering the variances

$$\sigma_n^2 := \left\langle \left(A_{nn} - \langle A_{nn} \rangle_V \right)^2 \right\rangle_V = \langle (A_{nn})^2 \rangle_V - \langle A_{nn} \rangle_V^2, \tag{14}$$

where $\langle ... \rangle_V$ indicates the average over the random perturbations V. In a first step (section 5.4), we will show that the mean values $\langle A_{nn} \rangle_V$ for sufficiently close n's differ very little in comparison to the experimental resolution limit δA introduced in section 2. In a second step (section 5.5), we will show that $\sigma_n \ll \delta A$, implying that A_{nn} differs very little from $\langle A_{nn} \rangle_V$ for most V. Altogether, this will imply the desired result that for most V's the A_{nn}'s change very little upon changing n (section 5.6).

To simplify the algebra, we henceforth assume that the largest and smallest eigenvalues of A in (1) satisfy

$$a_{\min} = -a_{\max}. \tag{15}$$

As a consequence, $a_{\max} = \Delta_A/2$ according to (1). Note that the assumption (15) does not imply any loss of generality, since adding an arbitrary constant (times the identity operator) to the observable A, and hence to all its eigenvalues, does not entail any non-trivial physical consequences. In particular, the above-mentioned changes of $\langle A_{nn} \rangle_V$ upon variation of n and the variances (14) remain exactly the same. For later use, we thus can conclude that

$$|\langle \psi | A^{\nu} | \psi \rangle| \leqslant (\Delta_A/2)^{\nu} \tag{16}$$

for any $\nu \in \mathbb{N}$.

For the sake of simplicity, we furthermore assume that all matrix elements V_{mn}^0 from (9) and U_{mn} from (10) are real numbers. For example, for systems without spins and magnetic fields, H_0 and V in (8) are both purely real operators in position representation and hence the eigenstates $|n\rangle_0$ and $|n\rangle$ can be chosen so that all V_{mn}^0 and U_{mn} become real. So, it is natural to assume that also the corresponding random matrix ensembles only involve real matrix elements. In particular, this implies with equations (13) and (14) that

$$\langle A_{nn} \rangle_V = \sum_{jk} A_{jk}^0 \left\langle U_{nj} U_{nk} \right\rangle_V \tag{17}$$

$$\sigma_n^2 = \sum_{ijkl} A_{ij}^0 A_{kl}^0 \left\langle U_{ni} U_{nj} U_{nk} U_{nl} \right\rangle_V - \langle A_{nn} \rangle_V^2. \tag{18}$$

It may well be that our subsequent calculations can be readily extended to systems for which such a transformation to purely real matrices V_{mn}^0 and U_{mn} is no longer possible. However, the so far available knowledge, e.g. from random matrix theory or numerical investigations, regarding the statistical properties of the U_{mn}'s is only sufficient for our purposes for real matrices (see next section). Since the subject of our paper is not the exploration of such statistical random matrix properties but rather their implications with respect to ETH, we confine ourselves to the case of real matrices.

5.3. Properties of U_{mn}

In view of (17), (18), some basic statistical properties of the matrix elements U_{mn} are needed in order to make any further progress.

At this point it is crucial to note that the Hamiltonian H in (8) gives rise to a very special type of random matrix. Namely, the matrix $_0\langle m | H | n \rangle_0$ is the sum of the above discussed random perturbation V_{mn}^0 and of the non-random diagonal matrix $_0\langle m | H_0 | n \rangle_0 = \delta_{mn} E_n^0$, whose diagonal elements E_n^0 grow approximately linearly with n (at least within a sufficiently small vicinity of the preset system energy E, onto which we tacitly restrict ourselves, see also sections 3 and 5.6). Out of the huge literature on random matrix theory, only a relatively small number of works pertains to this special case, see e.g. [46, 60, 62, 63] and further references therein. Strictly speaking, they are obtained for infinitely large matrices V_{mn}^0, whose statistical properties do not depend on m and n separately, but only on the difference $m - n$. Likewise, the unperturbed matrix $_0\langle m | H_0 | n \rangle_0$ is assumed to be infinitely large and of the form $\delta_{mn} E_n^0$ with equally spaced energy gaps $E_{n+1}^0 - E_n^0$. Intuitively, these seem quite plausible approximations, at least for not too strong perturbations V in (8). They can be readily justified by numerical examples, but somewhat more rigorous analytical results do not seem to exist. Here, we adopt the widely accepted viewpoint that, for out present purposes, they can be taken for granted [44, 60, 61].

As a consequence, also the statistical properties of the U_{mn} only depend on $m - n$, e.g. the νth moments are of the form

$$\langle (U_{mn})^\nu \rangle_V = u_\nu (m - n), \tag{19}$$

where the $u_\nu (n)$ are real (but not necessarily even [63]) functions of n, and are furthermore non-negative for even ν.

Known analytical results mainly concern the second moment $u_2 (n)$ for various ensembles of possibly banded and/or sparse random V-matrices, see e.g. [46, 60, 62, 63] and references therein. In all cases, it is found that $u_2 (n)$ is monotonically decreasing for $n \geqslant 0$ and monotonically increasing for $n \leqslant 0$, hence exhibiting a global maximum at $n = 0$:

$$\max_n \{ u_2 (n) \} = u_2 (0). \tag{20}$$

Since $\sum_k U_{mk} U_{nk} = \delta_{mn}$ we can conclude that

$$\sum_n u_2 (n) = 1, \tag{21}$$

implying that $u_2 (n)$ must approach zero for large $|n|$.

In all those analytical results, the mean values $\langle V_{mn}^0 \rangle_V$ are tacitly assumed to vanish and it is found that $u_2 (n)$ then only depends on the second moments $\langle (V_{mn}^0)^2 \rangle_V$. Since we are not aware of any justification for this assumption $\langle V_{mn}^0 \rangle_V = 0$, we have numerically investigated various examples and found that, indeed, the statistical properties of the U_{mn}'s seem to be independent of the first moments $\langle V_{mn}^0 \rangle_V$ (while keeping all other cumulants fixed). Furthermore, a simple physical argument is as follows: replacing an eigenstate $|n\rangle_0$ of H_0 by $-|n\rangle_0$ is supposed not to change any physically relevant properties of the given (non-random) model in (8). Note that this argument applies separately to any single n. Hence, it is quite plausible that upon randomly flipping the signs for half of all n's, the resulting 'new' V_{mn}^0's will be 'unbiased' for $m \neq n$. (More precisely: if a random matrix description works at all, then an ensemble with $\langle V_{mn}^0 \rangle_V = 0$ seems most appropriate). Finally, a possibly remaining systematic 'bias' of the diagonal elements V_{nn}^0 can be removed by adding an irrelevant constant to V. (The typical magnitude of the V_{mn}^0's is also estimated in Appendix B of [45], however, not taking into account the possibility that their average may be zero.)

For the rest, the detailed properties of $u_2 (n)$ are found—as expected—to still depend on the quantitative details of $\langle (V_{mn}^0)^2 \rangle_V$. Since no general statement about the latter seems possible for the general class of systems we have in mind with (8), we will focus on conclusions which do not depend on the corresponding details of $u_2 (n)$. Rather, we will only exploit the following very crude common denominator of all so far explored particular classes of random matrices V_{mn}, see e.g. [46, 60, 62, 63] and further references therein:

$$u_2 (0) = 10^{-O(N)}. \tag{22}$$

The basic physical reason is that exceedingly 'weak' perturbations V in (8) are tacitly ignored so that the smallest relevant energy scale is the mean level spacing $E_{n+1} - E_n$, being of the order of $10^{-O(N)}$ J according to section 2. Moreover, the ratio between this energy scale and any other relevant energy scale of the system can be very roughly estimated by $10^{-O(N)}$, independently of any further details of the specific model system in (8). As a consequence, the very crude estimate (22) is also independent of these details.

Further statistical properties of the U_{mn}, which we will, similarly as in [44, 45, 60, 62, 63], take for granted later on, are:

(i) Their average is zero, i.e.

$$u_1 (n) = 0 \quad \text{for all } n. \tag{23}$$

(ii) They are statistically independent of each other, i.e.

$$U_{mn} \text{ is independent of } U_{jk} \text{ if } m \neq j \text{ or } n \neq k. \tag{24}$$

(iii) Their distribution does not exhibit long tails, i.e.

$$u_4 (n) \leqslant c \, u_2 (n) u_2 (0) \quad \text{for all } n \tag{25}$$

with an n-independent constant c, which may possibly be very large but which is required not to be so large that it can compete in order of magnitude with $1/u_2 (0)$ from (22). For instance for a system with $N = 10^{23}$ particles, it would be sufficient that $c \leqslant 10^{10^{22}}$. In other words, we adopt the very weak assumption

$$c \, u_2 (0) = 10^{-O(N)}. \tag{26}$$

For example, for a Gaussian distribution (with zero mean, cf (23)) one finds that $u_4(n) = 3u_2^2(n)$ and hence (25) is satisfied for $c = 3$. Though a Gaussian distribution is often taken for granted [22, 44, 45], non-Gaussian distributions have been actually observed e.g. in [59] and also in our own numerical explorations (unpublished), but the more general condition (25) was still satisfied in all cases. We also note that since $u_2(n)/u_2(0)$ approaches zero for large $|n|$, the condition in (25) becomes weaker and weaker with increasing $|n|$.

5.4. Mean values

Evaluating (17) by means of (19), (23), and (24) yields

$$\langle A_{nn} \rangle_V = \sum_j A_{jj}^0 \left\langle U_{nj} U_{nj} \right\rangle_V + \sum_{j \neq k} A_{jk}^0 \left\langle U_{nj} \right\rangle_V \left\langle U_{nk} \right\rangle_V$$

$$= \sum_j A_{jj}^0 u_2(n - j). \tag{27}$$

It follows that

$$\Delta_n := \left\langle A_{n+1,n+1} \right\rangle_V - \left\langle A_{nn} \right\rangle_V$$

$$= \sum_j A_{jj}^0 \left[u_2(n + 1 - j) - u_2(n - j) \right] \tag{28}$$

and hence that

$$|\Delta_n| \leqslant \sum_j \left| A_{jj}^0 \right| \left| u_2(n + 1 - j) - u_2(n - j) \right|$$

$$\leqslant \max_j \left| A_{jj}^0 \right| \sum_k |u_2(k + 1) - u_2(k)|. \tag{29}$$

The maximum over j can be estimated from above by $\Delta_A/2$ according to (16). Recalling that $u_2(k)$ is monotonically decreasing for $k \geqslant 0$ and monotonically increasing for $k \leqslant 0$ (see above (20)), the sum over k amounts to $2 u_2(0)$ (more generally, this sum amounts to the total variation of $u_2(k)$; hence, if $u_2(k)$ exhibits M local maxima, it can be estimated from above by $2M \max_k u_2(k)$). Altogether, we thus can conclude that

$$\left| \left\langle A_{n+1,n+1} \right\rangle_V - \left\langle A_{nn} \right\rangle_V \right| \leqslant \Delta_A \, u_2(0). \tag{30}$$

This upper bound is tight: one can readily find examples A for which (30) becomes an equality. Moreover, it follows that

$$\left| \left\langle A_{mm} \right\rangle_V - \left\langle A_{nn} \right\rangle_V \right| \leqslant |m - n| \, \Delta_A \, u_2(0). \tag{31}$$

By generalizing the line of reasoning in (29), (30) one can also show that

$$\left| \left\langle A_{mm} \right\rangle_V - \left\langle A_{nn} \right\rangle_V \right| \leqslant \Delta_A \sum_{k=-\kappa}^{\kappa} u_2(k) \tag{32}$$

with $\kappa := |m - n| - 1$. Under certain conditions, the bound (31) may be better than (32), but never by more than a factor of 2. For sufficiently large $|m - n|$, (32) is always better since the sum on the right-hand side is bounded by unity (see (21)), while the right-hand side of (31) is unbounded. (The relevance of large $|m - n|$-values will become apparent in section 5.6 below). In any case, (32) is a rather tight bound in the sense that one can find examples for A_{jj}^0 so that the left-hand side is larger than the right-hand side divided by 2 for a set of suitably chosen pairs (m, n) so that the differences $m - n$ may still take any integer value.

5.5. Variances

We rewrite the variance from (18) as

$$\sigma_n^2 + \langle A_{nn} \rangle_V^2 = \sum_{ijkl} A_{ij}^0 A_{kl}^0 \left\langle U_{ni} U_{nj} U_{nk} U_{nl} \right\rangle_V \tag{33}$$

and evaluate the four-fold sum by distinguishing four possible cases. Case 1: $i \neq k$ and $i = j$. In this case, we only have to keep summands with $l = k$: otherwise the factor U_{nk} on the right-hand side of (33) would be independent of the remaining three factors according to (24), and the corresponding summand would vanish according to (19) and (23). Case 2: $i \neq k$ and $i \neq j$. As before, we can conclude that only summands with $l = i$ and $j = k$ give rise to non-vanishing terms. Case 3: $i = k$ and $i \neq l$, implying, as before, that only $j = l$ contribute. Case 4: $i = k$ and $i = l$, implying $j = i$. Consequently, we can rewrite (33) as

$$\sigma_n^2 + \langle A_{nn} \rangle_V^2 = \Sigma_1 + \Sigma_2 + \Sigma_3 + \Sigma_4, \tag{34}$$

where the four summands correspond to the above four cases and can be rewritten as:

$$\Sigma_1 = \sum_{i \neq k} A_{ii}^0 A_{kk}^0 \langle U_{ni} U_{ni} U_{nk} U_{nk} \rangle_V, \tag{35}$$

$$\Sigma_2 = \sum_{i \neq k} A_{ik}^0 A_{ki}^0 \langle U_{ni} U_{nk} U_{nk} U_{ni} \rangle_V, \tag{36}$$

$$\Sigma_3 = \sum_{i \neq l} A_{il}^0 A_{il}^0 \langle U_{ni} U_{nl} U_{ni} U_{nl} \rangle_V, \tag{37}$$

$$\Sigma_4 = \sum_i A_{ii}^0 A_{ii}^0 \langle U_{ni} U_{ni} U_{ni} U_{ni} \rangle_V. \tag{38}$$

With the help of (24) and (19) we can rewrite (35) as

$$\begin{aligned}
\Sigma_1 &= \sum_{i \neq k} A_{ii}^0 A_{kk}^0 u_2(n - i) u_2(n - k) \\
&= \sum_{ik} A_{ii}^0 A_{kk}^0 u_2(n - i) u_2(n - k) - \sum_i (A_{ii}^0)^2 u_2^2(n - i) \\
&= \langle A_{nn} \rangle_V^2 - \sum_i (A_{ii}^0)^2 u_2^2(n - i),
\end{aligned} \tag{39}$$

where we exploited (27) in the last equation. Likewise, one finds that

$$\Sigma_2 = \sum_{ik} |A_{ik}^0|^2 u_2(n - i) u_2(n - k) - \sum_i (A_{ii}^0)^2 u_2^2(n - i), \tag{40}$$

$$\Sigma_3 = \sum_{il} (A_{il}^0)^2 u_2(n - i) u_2(n - l) - \sum_i (A_{ii}^0)^2 u_2^2(n - i), \tag{41}$$

$$\Sigma_4 = \sum_i (A_{ii}^0)^2 u_4(n - i). \tag{42}$$

Introducing these results into (34) thus yields

$$\sigma_n^2 = S_1 + S_2 + S_3, \tag{43}$$

$$S_1 := \sum_{ik} |A_{ik}^0|^2 u_2(n - i) u_2(n - k), \tag{44}$$

$$S_2 := \sum_{il} (A_{il}^0)^2 u_2(n - i) u_2(n - l), \tag{45}$$

$$S_3 := \sum_i (A_{ii}^0)^2 [u_4(n - i) - 3u_2^2(n - i)]. \tag{46}$$

The three factors on the right-hand side of (44) are all non-negative and hence

$$S_1 = |S_1| \leqslant \max_k \{u_2(k)\} \sum_i u_2(n - i) \sum_k A_{ik}^0 A_{ki}^0. \tag{47}$$

With (11) one readily sees that the last sum over k amounts to $_0\langle i|A^2|i\rangle_0 =: (A^2)_{ii}^0$. Exploiting (20) we thus obtain

$$S_1 \leqslant u_2(0) \sum_i (A^2)_{ii}^0 \, u_2(n - i). \tag{48}$$

Likewise, since $u_2(i) \geqslant 0$ for all i, the modulus of (45) can be estimated as

$$|S_2| \leqslant \sum_{il} |A_{il}^0|^2 u_2(n - i) u_2(n - l) = S_1. \tag{49}$$

Turning to (46), we first note that the last factor $\kappa_4 := u_4(n - i) - 3u_2^2(n - i)$ represents the 4th cumulant of the random variable U_{ni}. For a Gaussian distribution (the case considered by Deutsch [44, 45]), this cumulant vanishes, but for more general distributions it may be finite and of either sign. We thus estimate $|\kappa_4|$ from above by $u_4(n - i) + 3u_2^2(n - i)$. Observing (26) and $u_2^2(n - i) \leqslant u_2(0) u_2(n - i)$ (see (20)), we thus can bound (46) by

$$|S_3| \leqslant u_2(0)(c + 3) \sum_i (A_{ii}^0)^2 u_2(n - i). \tag{50}$$

Next, we invoke the Cauchy–Schwarz inequality to conclude

$$\langle \psi | B | \psi \rangle^2 \leqslant \langle \psi | \psi \rangle \langle \psi | B^2 | \psi \rangle \tag{51}$$

for arbitrary Hermitian operators B and vectors $|\psi\rangle$. In particular, it follows that $(A_{ii}^0)^2 \leqslant (A^2)_{ii}^0$. Altogether, we thus arrive at

$$\sigma_n^2 \leqslant (c + 5)\, u_2(0) \sum_i (A^2)_{ii}^0\, u_2(n - i).$$ (52)

Finally, we exploit (16) and (21), resulting in

$$\sigma_n^2 \leqslant (c + 5)\, u_2(0)\, (\Delta_A/2)^2 = 10^{-\mathrm{O}(N)}\, \Delta_A^2,$$ (53)

where we used (26) in the last step.

5.6. Discussion

From (14), (53), and Markov's inequality it follows that

$$\mathrm{Prob}\left(\left| A_{nn} - \langle A_{nn}\rangle_V \right| \geqslant \epsilon\right) \leqslant (\Delta_A/\epsilon)^2\, 10^{-\mathrm{O}(N)}$$ (54)

for any $\epsilon > 0$, where Prob (X) denotes the probability that a randomly sampled V in (8) entails property X. For instance, if in the last term $\mathrm{O}(N) = 10^{23}$ and $\epsilon = \Delta_A\, 10^{-10^{22}}$ then the right-hand side of (54) is still $10^{-\mathrm{O}(10^{23})}$. Consequently, the joint probability that every A_{nn} is practically indistinguishable from $\langle A_{nn}\rangle_V$ simultaneously for all $n \in \{n_0, .., n_0 + \Delta n\}$ still remains negligibly small if $0 \leqslant \Delta n \ll 10^{\mathrm{O}(N)}$.

On the other hand, (22) and (31) imply that the difference $\langle A_{mm}\rangle_V - \langle A_{nn}\rangle_V$ remains below the experimental resolution limit δA of A (cf section 2) even for quite large range-to-resolution ratios $\Delta_A/\delta A$, provided $|m - n|$ remains much smaller than of the order of $10^{\mathrm{O}(N)}$. In other words, the variations of the $\langle A_{nn}\rangle_V$ also remain negligibly small within the 'window' of n-values $\{n_0, .., n_0 + \Delta n\}$ if $0 \leqslant \Delta n \ll 10^{\mathrm{O}(N)}$.

Altogether, we thus arrive at the conclusion that for the vast majority of randomly sampled perturbations V in (8), the A_{nn}'s remain practically constant (below the experimental resolution limit) as long as n varies by much less than $10^{\mathrm{O}(N)}$.

The latter property is sometimes referred to as the strong ETH [33, 38]. It immediately implies the practical indistinguishability of the two expectation values (6) and (7), and hence thermalization, provided both the $\rho_{nn}(0)$ and the ρ_{nn}^{mic} are negligibly small outside a window of n-values much smaller than $10^{\mathrm{O}(N)}$, but otherwise without any further restriction on the initial condition $\rho(0)$.

If the range Δn of admitted n-values is not any more much smaller than $10^{\mathrm{O}(N)}$, then we can no longer conclude from (53) that with high probability all the A_{nn}'s remain simultaneously close to the $\langle A_{nn}\rangle_V$'s. However, we still can conclude that for the vast majority of n's, those differences remain negligibly small[2]. If, in addition, the variations of the $\langle A_{nn}\rangle_V$'s would remain small, we still could conclude that 'most' A_{nn}'s are practically equal (for the overwhelming majority of V's), i.e. the so-called weak ETH is satisfied [33, 38]. As a consequence, the expectation values (6) and (7) would again be practically equal under certain additional conditions on the initial condition $\rho(0)$. For instance, the total weight of all $\rho_{nn}(0)'s$ corresponding to exceptionally large differences $A_{nn} - \langle A_{nn}\rangle_V$ should remain sufficiently small. For example (4) would obviously be a sufficient condition.

However, this line of reasoning contains a problem: if the variations Δn of n are not any more much smaller than $10^{\mathrm{O}(N)}$, then equations (31) and (22) no longer imply that the variations of $\langle A_{nn}\rangle_V$ remain negligible. The same conclusion follows from the bound (32). Since the latter bound is already rather tight (see below (32)), we can conclude that the restriction to windows of n-values much smaller than $10^{\mathrm{O}(N)}$ is not merely a technical problem but rather an indispensable prerequisite of the random matrix model from section 5.1. In particular, this restriction also concerns the original findings by Deutsch [44].

Note that Δn from above is identical to the number D of energy eigenvalues E_n contained in the microcanonical energy window $I_{\mathrm{mic}} := [E - \Delta E, E]$ from section 3. The above discussed restriction thus amounts to

$$D \ll 10^{\mathrm{O}(N)}$$ (55)

and implies that ΔE must remain very much smaller than any macroscopically resolvable energy difference. (This follows from the fact that the energy eigenstates are exponentially dense in the system size N, see section 2).

6. Srednicki's ETH for the off-diagonal matrix elements

In [23, 24], Srednicki formulated, besides the so far considered ETH for the diagonal matrix elements A_{nn}, also a corresponding ETH for the off-diagonal elements A_{mn} with $m \neq n$. This hypothesis can also be readily confirmed within our present framework:

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[2] With $x_n := |A_{nn} - \langle A_{nn}\rangle_V|$ and $\delta := (\Delta_A/\epsilon)^2\, 10^{-\mathrm{O}(N)}$, equation (54) can be rewritten as $\langle \Theta(x_n - \epsilon)\rangle_V \leqslant \delta$, where $\Theta(x)$ is the Heaviside step function. Furthermore, $Z_\epsilon := \sum_{n=1}^D \Theta(x_n - \epsilon)$ counts how many of the x_n's exceed ϵ. It follows that $\langle Z_\epsilon\rangle_V \leqslant D\,\delta$ and with Markov's inequality that Prob $(Z_\epsilon \geqslant qD) \leqslant \delta/q$, where Prob $(Z_\epsilon \geqslant qD)$ is the probability that more than a fraction q of all x_n's exceed ϵ.

similarly as in (17), we find from (13) that

$$\langle A_{mn} \rangle_V = \sum_{jk} A_{jk}^0 \langle U_{mj} U_{nk} \rangle_V. \tag{56}$$

For $m \neq n$, the last factor $\langle U_{mj} U_{nk} \rangle_V$ equals $\langle U_{mj} \rangle_V \langle U_{nk} \rangle_V$ according to (24), and hence vanishes according to (19) and (23). In conclusion

$$\langle A_{mn} \rangle_V = 0 \tag{57}$$

for all $m \neq n$.

Turning to the second moment (variance), one finds similarly as in (14), (18) that

$$\langle |A_{mn}|^2 \rangle_V = \langle A_{mn} A_{nm} \rangle_V = \sum_{ijkl} A_{ij}^0 A_{kl}^0 \langle U_{mi} U_{nj} U_{nk} U_{ml} \rangle_V. \tag{58}$$

According to (24), for $m \neq n$ the last term $\langle U_{mi} U_{nj} U_{nk} U_{ml} \rangle_V$ now factorizes into $\langle U_{mi} U_{ml} \rangle_V \langle U_{nj} U_{nk} \rangle_V$. Exploiting (24) once more implies $\langle U_{mi} U_{ml} \rangle_V = \delta_{il} \langle U_{mi}^2 \rangle_V$ and $\langle U_{nj} U_{nk} \rangle_V = \delta_{jk} \langle U_{nk}^2 \rangle_V$. With (19) we thus obtain

$$\langle |A_{mn}|^2 \rangle_V = \sum_{ik} |A_{ik}^0|^2 u_2(m-i) u_2(n-k). \tag{59}$$

Step by step as in (44), (47), (48), (53) it follows that

$$\langle |A_{mn}|^2 \rangle_V \leqslant u_2(0)(\Delta_A/2)^2 \tag{60}$$

for all $m \neq n$. In view of (22) we see that the off-diagonals $|A_{mn}|$ are typically exponentially small in the system size N, in agreement with Srednicki's prediction in [23, 24].

The overall conclusion applying to any given Hermitian operator A of finite range Δ_A is: the representation of A in the eigenbasis of H is, for the overwhelming majority of randomly sampled perturbations V in (8), very close to a diagonal matrix, whose diagonal elements A_{nn} change very slowly with n.

7. Implications for the level populations $\rho_{nn}(0)$

Throughout this section, we consider the density operator $\rho(0)$ (pure or mixed state) from section 2 and abbreviate it as ρ.

Since ρ is a Hermitian operator, all results so far for general observables A are immediately applicable to ρ. However, this particular observable $A = \rho$ also exhibits some subtle special features. Therefore, we first focus on a simple example.

7.1. Simple example

We consider a pure energy eigenstate of the unperturbed Hamiltonian H_0 in (8), i.e.

$$\rho = |m\rangle_0 \, {}_0\langle m| \tag{61}$$

with an arbitrary but fixed m. Its eigenvalues are either zero or one, hence the range from (1) is $\Delta_\rho = 1$. Observing that $\rho_{ik}^0 = \delta_{im} \delta_{km}$ it follows from (13) and (17) to (19) that

$$\rho_{nn} = |U_{mn}|^2, \tag{62}$$

$$\langle \rho_{nn} \rangle_V = u_2(n-m), \tag{63}$$

$$\sigma_n^2 = u_4(n-m) - u_2^2(n-m), \tag{64}$$

where the variance from (14) is given for $A = \rho$ by

$$\sigma_n^2 := \left\langle (\rho_{nn})^2 \right\rangle_V - \left\langle \rho_{nn} \right\rangle_V^2. \tag{65}$$

As a concrete example, we may focus on Gaussian distributed U_{mn}'s (see below equation (26)), so that $u_4(n) = 3u_2^2(n)$ and hence

$$\sigma_n^2 = 2 u_2^2(n-m). \tag{66}$$

Altogether, the standard deviation σ_n of the random variable ρ_{nn} from (62) is thus comparable to its mean value $\langle \rho_{nn} \rangle_V$, and both are, according to (20) and (22), extremely small compared to the range $\Delta_\rho = 1$ of the considered observable ρ. Within any reasonable resolution limit $\delta\rho$ of this observable we thus can conclude that, for the vast majority of random perturbations V in (8), all ρ_{nn}'s are practically equal (namely zero), in agreement with the general validation of ETH from section 5. But for our present purposes, this usual resolution limit $\delta\rho$ is

still way too large. On the actual scale of interest, the ρ_{nn}'s from (62) are not at all a slowly varying function of n, but rather exhibit very significant random fluctuations (see also (24)). In particular, it would be wrong to argue that the $\rho_{nn}(0)$'s in (7) are now practically constant and hence, upon comparison with (6), thermalization follows.

7.2. General case

We return to general density operators ρ, i.e., we only assume that ρ is a Hermitian, non-negative operator of unit trace and purity

$$\text{Tr}\{\rho^2\} \leqslant 1. \tag{67}$$

In the following, we will exploit these properties of ρ, which, however, would be lost after adding a constant to ρ so that (15) is satisfied. Hence we only can employ those previous results which were obtained without the help of (15). Along these lines, one finds exactly as in (27) and (52) that

$$\langle \rho_{nn} \rangle_V = \sum_j \rho_{jj}^0 u_2(n-j), \tag{68}$$

$$\sigma_n^2 \leqslant (c+5) u_2(0) \sum_i (\rho^2)_{ii}^0 u_2(n-i), \tag{69}$$

where σ_n^2 is defined in (65) and $(\rho^2)_{ii}^0 := {}_0\langle i| \rho^2 |i\rangle_0$. Likewise, (57) and (59) yield

$$\langle \rho_{mn} \rangle_V = 0, \tag{70}$$

$$\left\langle |\rho_{mn}|^2 \right\rangle_V = \sum_{ik} |\rho_{ik}^0|^2 u_2(m-i) u_2(n-k) \tag{71}$$

for all $m \neq n$.

Introducing (20) into (68) implies

$$\langle \rho_{nn} \rangle_V \leqslant \max_j \{u_2(j)\} \sum_j \rho_{jj}^0 = u_2(0), \tag{72}$$

where we exploited that the sum over j equals $\text{Tr}\,\rho = 1$. Likewise, (69) yields

$$\sigma_n^2 \leqslant (c+5) u_2^2(0)\, \text{Tr}\{\rho^2\}. \tag{73}$$

Rewriting the definition from (28) as

$$\Delta_n := \langle \rho_{n+1,n+1} \rangle_V - \langle \rho_{nn} \rangle_V \tag{74}$$

we find along similar lines of reasoning that

$$\begin{aligned}
|\Delta_n| &\leqslant \sum_j \rho_{jj}^0 |u_2(n+1-j) - u_2(n-j)| \\
&\leqslant \max_n |u_2(n+1) - u_2(n)|.
\end{aligned} \tag{75}$$

Moreover, we can conclude that

$$\sum_n |\Delta_n| \leqslant \sum_j \rho_{jj}^0 \sum_n |u_2(n+1-j) - u_2(n-j)|. \tag{76}$$

Similarly as in (30), the last sum is seen to be equal to $2\,u_2(0)$. The remaining sum over j equals $\text{Tr}\,\rho = 1$ and hence

$$\sum_n |\Delta_n| \leqslant 2\,u_2(0). \tag{77}$$

Equations (72), (73) indicate that, in contrast to pure states in (61), for mixed states of small purity $\text{Tr}\{\rho^2\}$, the random fluctuations of the ρ_{nn}'s about their mean values may become negligible. Moreover, the right-hand side of (75) usually turns out [44, 45, 60, 62, 63] to be of the order of $u_2^2(0)$. The same conclusion is also suggested by (77). Consequently, also the variations of $\langle \rho_{nn} \rangle_V$ as a function of n become small. Unlike for pure states we thus can now conclude that (6) and (7) are approximately equal, implying thermalization. However, assuming a small purity of ρ represents a quite strong restriction in the first place.

Returning to general ρ, we can deduce from (20) and (68) that

$$\sum_n \left\langle \rho_{nn} \right\rangle_V^2 \leqslant \sum_n \max_j \{ u_2(j) \} \sum_j \rho_{jj}^0 \sum_k \rho_{kk}^0 u_2(n-k)$$
$$\leqslant u_2(0) \sum_j \rho_{jj}^0 \sum_k \rho_{kk}^0 \sum_n u_2(n-k). \tag{78}$$

The sum over n equals one according to (21) and the two remaining sums are equal to $\mathrm{Tr}\, \rho = 1$, i.e.

$$\sum_n \left\langle \rho_{nn} \right\rangle_V^2 \leqslant u_2(0). \tag{79}$$

Likewise, equations (67) and (69) imply

$$\sum_n \sigma_n^2 \leqslant (c+5) u_2(0) \sum_i (\rho^2)_{ii}^0 \sum_n u_2(n-i)$$
$$= (c+5) u_2(0) \mathrm{Tr}\{\rho^2\} \leqslant (c+5) u_2(0). \tag{80}$$

Altogether, this yields

$$\sum_n \left\langle (\rho_{nn})^2 \right\rangle_V \leqslant (c+6) u_2(0) \tag{81}$$

and with (25)

$$\left\langle \sum_n (\rho_{nn})^2 \right\rangle_V \leqslant 10^{-\mathrm{O}(N)}. \tag{82}$$

Since $(\max_n \rho_{nn})^2 = \max_n (\rho_{nn})^2 \leqslant \sum_n (\rho_{nn})^2$ it follows that

$$\left\langle \left(\max_n \{\rho_{nn}\} \right)^2 \right\rangle_V \leqslant 10^{-\mathrm{O}(N)} \tag{83}$$

and hence by Markov's inequality that

$$\mathrm{Prob}\left(\max_n \{\rho_{nn}\} \geqslant \epsilon \right) \leqslant \epsilon^{-2} \, 10^{-\mathrm{O}(N)}, \tag{84}$$

see also the explanations below (54).

7.3. Off-diagonals

We focus on the off-diagonal matrix elements ρ_{mn} with $m \neq n$. Their mean values are zero according to (70). Their variance can be readily bounded by the Cauchy–Schwarz inequality

$$\left| \rho_{mn} \right|^2 \leqslant \rho_{mm} \, \rho_{nn}. \tag{85}$$

Likewise, introducing $|\rho_{ik}^0|^2 \leqslant \rho_{ii}^0 \rho_{kk}^0$ into (71) yields with (68) the estimate

$$\left\langle \left| \rho_{mn} \right|^2 \right\rangle_V \leqslant \left\langle \rho_{mm} \right\rangle_V \left\langle \rho_{nn} \right\rangle_V. \tag{86}$$

Similarly as below (47) one sees that $\sum_{mn} |\rho_{mn}|^2 = \mathrm{Tr}\{\rho^2\}$ and hence

$$\sum_{m \neq n} \left\langle \left| \rho_{mn} \right|^2 \right\rangle_V = \mathrm{Tr}\{\rho^2\} - \left\langle \sum_n \rho_{nn}^2 \right\rangle_V \leqslant \mathrm{Tr}\{\rho^2\}. \tag{87}$$

According to (82), the last inequality in (87) is in fact a very tight upper bound. The same estimate follows by summing in (71) over m and n. Neither of these results indicate that the off-diagonal matrix elements are typically much smaller than the diagonal elements. We thus conjecture that typical off-diagonal matrix elements will in fact not be small compared to the diagonal elements. Trivial exceptions are pure states (61). Non-trivial exceptions may be mixed states of low purity, similarly as below (77).

7.4. Discussion

The main result of this section is (84): it implies that for the overwhelming majority of randomly sampled perturbations V in (8) the last term in (3) is unimaginably small (essentially in agreement with (4)). In other words, equilibration in the sense of section 2 is verified. We emphasize that all these conclusions do not depend an any further details of the actual initial condition $\rho(0)$, except that it is assumed to be fixed, i.e. independent of the randomly sampled V.

The physical interpretation is as follows: one specific, usually not very well known, but nevertheless well-defined initial state $\rho(0)$ (pure or mixed) is 'given' to us, and then evolves further in time according to one particular, randomly picked system Hamiltonian (8). Our results guarantee that the vast majority of those randomly sampled Hamiltonians gives rise to equilibration in the sense of equation (3). As the only unproven part remains the assumption that the actual (in detail not exactly known) system does not correspond to one of the rare, untypical Hamiltonians of the considered random ensemble.

Since $\mathrm{Tr}\{\rho\} = \sum_n \rho_{nn} = 1$ we can conclude from (84) that, for most V's, the number of non-negligible ρ_{nn}'s *cannot* be much smaller than $10^{O(N)}$. As a consequence, the strong ETH scenario from section 5.6 does not apply. In turn, to apply this scenario, a different physical set up is required, with a different physical view of how the initial condition ρ arises. Namely, one particular, but 'typical' V in (8) is considered to have been randomly sampled but now is held fixed. Since we assumed the system is typical, strong ETH as specified in section 5.6 can and will be taken for granted. In a next step, the initial state $\rho = \rho(0)$ for this particular system is specified, arising, e.g., as the result of an experimental preparation procedure for this very system (with respect to other systems H of the ensemble, this preparation procedure may not be physically meaningful or not even well defined). Finally, there must be good reasons (e.g. a very careful experimentalist) to assume that this preparation process yields level populations ρ_{nn} which are negligible outside a window of n-values much smaller than $10^{O(N)}$, see equation (55).

In conclusion, our present formalism is able to validate either equilibration or thermalization, but not both of them simultaneously for one and the same physical model system.

8. Comparison with the approach by Goldstein and coworkers

In a series of works [5, 13, 16, 47, 48] Goldstein and coauthors addressed the problem of thermalization by means of an approach which, at first glance, seems to be entirely different from our present one. In particular, the 'intermediate' problem of equilibration (see section 2) apparently can be entirely circumvented. One key point of their approach is the restriction to so-called macroscopic observables, i.e. observables whose statistical fluctuations are negligibly small for macroscopic systems at thermal equilibrium. In this section, we will show that the latter defining property of a macroscopic observable implies that it satisfies (weak) ETH. In other words, the restriction to such observables is essentially equivalent to assuming ETH.

We define the microcanonical mean and variance of any given observable A as

$$\overline{A} := \mathrm{Tr}\{\rho_{\mathrm{mic}}\, A\}, \tag{88}$$

$$\Delta A^2 := \mathrm{Tr}\{\rho_{\mathrm{mic}}\, (A - \overline{A})^2\}, \tag{89}$$

where ρ_{mic} is the microcanonical ensemble from (5). By definition, an observable A is called a *macroscopic observable*, if its fluctuations ΔA are negligibly small. A more precise formal requirement would be vanishing fluctuations in the thermodynamic limit. A more appropriate real world (experimentally useful) version would be to require that the fluctuations are smaller than the experimental resolution limit δA, with, e.g. $\delta A = 10^{-10}\Delta_A$, where Δ_A is the measurement range of the experimental instrument modelled by A, see section 2.

The above requirement represents a minimal condition: whatever alternative definition of a macroscopic observable may be proposed, if it admits non-small fluctuations in the microcanonical ensemble then it would not seem well-defined to us. Indeed, the definitions employed in [5, 13, 16] are quite similar but not exactly identical to ours. We also note that the microcanonical ensemble itself is only used here as a formal device to define the notion of a macroscopic observable. It does not in any way anticipate that the actual system of interest should exhibit thermalization.

Introducing (5) into (88) and (89) implies

$$\overline{A} = \frac{1}{D}\sum_{\mathrm{mic}} A_{nn}, \tag{90}$$

$$\Delta A^2 = \frac{1}{D}\sum_{\mathrm{mic}} (A^2)_{nn} - (\overline{A})^2, \tag{91}$$

where $(A^2)_{nn} := \langle n\,|A^2|\,n\rangle$. In other words, (90) represents the average over those A_{nn}'s, whose energies E_n are contained in the microcanonical energy window. Their typical deviation from this average is quantified by the variance

$$\Delta A_{\mathrm{ETH}}^2 := \frac{1}{D}\sum_{\mathrm{mic}} (A_{nn} - \overline{A})^2 = \frac{1}{D}\sum_{\mathrm{mic}} (A_{nn})^2 - (\overline{A})^2. \tag{92}$$

From (51) we can conclude that $(A_{nn})^2 \leqslant (A^2)_{nn}$ and hence that $\Delta A_{ETH} \leqslant \Delta A$. Assuming that A is a macroscopic observable thus implies that ΔA_{ETH} is small [33]. According to the definition in (92) it follows that most A_{nn}'s must be close to $\overline{A}$, i.e. weak ETH is satisfied (see section 5.6).

Closely related considerations are originally due to [33], however focusing on so-called intensive local few-body operators rather than on macroscopic observables.

Restricting oneself to macroscopic observables clearly has a long and well founded tradition, especially with respect to the thermodynamic roots of statistical physics. On the other hand, statistical physics itself is by no means restricted to such observables. Rather, it is understood and experimentally (and numerically) seen that also 'microscopic' observables are perfectly well described by this theory. Such observables exhibit non-negligible fluctuations about their mean values and as such are hardly encountered in our everyday macroscopic world (exceptions may arise near critical points). But already with the help of an optical microscope, interesting observables exhibiting non-negligible thermal fluctuations (e.g. Brownian motion) become accessible. Even more so, within the rapidly developing fields of nanotechnology and single molecule experiments, such microscopic observables become of increasing practical relevance.

We finally remark that Goldstein and coworkers conceive their own approach [5, 13, 16, 47, 48] as a continuation of von Neumann's ground-breaking work [49]. Other relations between such an approach and ETH than the one discussed above have also been pointed out in [36, 48]. Furthermore, the concept of randomized Hamiltonians (or random matrices) also plays a key role in the approach by von Neumann and by Goldstein and coworkers [47]. However, rather than introducing this randomness directly into the Hamiltonian H itself—as done in the approach by Deutsch via equation (8)—the randomness is now introduced by prescribing the statistical properties of the randomly sampled eigenbases $|n\rangle$ of H, see section 5.2, while keeping the spectrum of H fixed. In spite of these technical differences, the two approaches are thus in fact very close in spirit (see, e.g. section 6 in [47]).

9. Summary and conclusions

In a first step, we reconsidered the random matrix model of Deutsch [44–46] and worked out a more detailed and slightly more general demonstration that it validates ETH: for the overwhelming majority of the corresponding random ensemble of Hamiltonians H, any given observable A is represented in the eigenbasis of H by an almost diagonal matrix with very slowly varying diagonal elements. More precisely: apart from a fraction of exceptional H's which is exponentially small in the system size N, the off-diagonal matrix elements A_{mn} are exponentially small in N and the changes of the diagonal elements A_{nn} as a function of n are also exponentially small in N. This implies the following solution of problem (i) from section 4: for any given H, one can readily construct (*a posteriori*) an ETH-violating A (see section 4), but any such A still continues to satisfy ETH for most other H's. In turn, if H is not known in all details with extremely high precision, then a given observable is exceedingly likely to exhibit ETH.

The generalization for more than one observable is straightforward: given every single observable is exponentially unlikely to violate ETH, it is still extremely likely that all of them will simultaneously exhibit ETH, as long as their number is not exponentially large, i.e. remains within the limits of what is feasible in any real (or numerical) experiment.

In a second step, we have shown by means of a further generalization of Deutsch's approach that also an essential prerequisite for equilibration, namely equation (4), will be satisfied for the overwhelming majority of Hamiltonians H. In doing so, an arbitrary (pure or mixed) state $\rho(0)$ is admitted as initial condition. But this initial state $\rho(0)$ must then remain always the same for the entire ensemble of random Hamiltonians H.

We also identified a not yet satisfactorily solved aspect of Deutsch's original approach and our present generalization: on the one hand, the changes of the diagonal matrix elements A_{nn} as a function of n are exponentially small in the system size N up to exponentially rare exceptions. On the other hand, the typical difference between neighbouring energy levels E_n is also exponentially small in N (cf section 2), i.e. the number of energy eigenvalues contained in an energy intervals $[E - \Delta E, E]$ is exponentially large in N for the usual ΔE's of interest. Hence, the variations of A_{nn} within the entire energy interval may no longer be negligible. As a consequence, thermalization, i.e., the practical indistinguishability of (6) and (7), can only be proven under the extra condition that the interval of relevant n-values, which notably contribute to those sums in (6) and (7), is not too large, namely much smaller than $10^{O(N)}$ (cf (55)). In other words, only exceedingly small ΔE's are admitted. In the following four paragraphs, we conclude with four noteworthy remarks and implications.

In spite of this restriction, the admitted range of n-values is still huge, and likewise for the admitted energy intervals ΔE in comparison with the energy level spacings. In particular, they are still of physical interest: for instance, one may imagine that the experimentalist has prepared the system with a sufficiently small uncertainty

in the total system energy E so that the corresponding condition can be safely taken for granted for the ρ_{nn}'s appearing in (6) and (7).

As mentioned already in in section 4, our findings imply the equivalence of ρ_{eq} in (7) not only with the microcanonical ensemble ρ_{mic} in (6) but also with any other equilibrium (i.e. steady state) ensemble, provided that its level populations are mainly concentrated within a sufficiently small energy window as specified above. Unfortunately, this condition is not satisfied e.g. for the canonical ensemble.

The other, more fortunate side of the coin is that within our present approach the diagonal matrix elements A_{nn} are indeed *not* forbidden to exhibit non-negligible variations for sufficiently large changes of n, or, equivalently, for macroscopically notable changes of E_n. This solves problem (ii) from section 4.

Assuming one and the same initial state $\rho(0)$ for the entire ensemble of random Hamiltonians H, as done in our above discussion of equilibration, implies that the number of ρ_{nn}'s which notably contribute in (7) is *not* much smaller than $10^{O(N)}$ for most H's. In conclusion, our present generalization of Deutsch's approach allows us to corroborate either equilibration or thermalization, but not both of them simultaneously for one and the same physical model system. The root of the problem is as before: whether and why the dependence of the diagonal matrix elements A_{nn} on n is neither too strong nor too weak is not yet fully satisfactorily understood. A solution of this problem is currently being worked out.

Acknowledgments

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