Mechanism of slow equilibration of isolated quantum systems

Anatoly Dymarsky

Department of Physics and Astronomy,
University of Kentucky, Lexington, KY 40506 and
Skolkovo Institute of Science and Technology,
Skolkovo Innovation Center, Moscow, Russia, 143026

(Dated: February 28, 2022)

We discuss the approach toward equilibrium of an isolated quantum system. For a wide class of systems we argue that the time-averaged expectation value of a local operator in any initial state is bounded by the so-called deviation function, which characterizes maximal deviation from the equilibrium for all states with a given value of energy fluctuations. We provide numerical evidence that the bound is approximately saturated by the initial configurations with spatial inhomogeneities at macroscopic level. In this way the deviation function establishes an explicit connection between the macroscopically observed timescales associated with transport and properties of microscopic matrix elements. The form of the deviation function indicates that among the slowest states which saturate the bound there are also those with arbitrarily long equilibration times.

Emergence of statistical mechanics for isolated quantum systems has been an active topic of research for the last decade. While thermodynamic equilibrium of a quantum many-body system can be successively explained using typicality arguments [1][3], to quantitatively describe the approach towards equilibrium proved to be a far more challenging task. Eventual equilibration of quantum systems was proved under a wide range of conditions in [4–10] (also see [11, 12] for reviews), but the resulting uniform bound on equilibration timescales established so far is exponential in system size [13]. Clearly, this is not the timescales observed macroscopically. At the same time much stronger bounds independent of system size were found for the special initial conditions or observables, either typical in a technical sense or with low entanglement, etc. [14][21]. These results can explain local pre-thermalization of quantum system, but fail short of describing late time dynamics normally associated with transport. In the latter case characteristic timescales normally grow polynomially with the system size. In this paper we elucidate the mechanism of slow equilibration, when characteristic times grow with the system size, and identify relevant timescales microscopically, starting from the underlying quantum-mechanical description.

In this work we consider equilibration from the point of view of an observable. It is known that there are always artificial observables which require exponentially long in system size time to thermalize [14][22]. Our focus instead is on the physically motivated observables, such as macroscopic averaged or local observables which are expected to equilibrate at most in polynomial time.

We assume that the quantum system under consideration has a discrete spectrum of energies $E_i$ and corresponding eigenstates $|E_i\rangle$. As a technical assumption which can be relaxed we assume the spectrum is non-degenerate. The initial states $\Psi$ will belong to a microcanonical interval specified by a mean energy $E_\Psi$ and width $2\Delta E_\Psi$,  

$$|\Psi\rangle = \sum_i c_i |E_i\rangle, \quad E_i \in [E_\Psi - \Delta E_\Psi, E_\Psi + \Delta E_\Psi].$$  

For the given initial $\Psi$ equilibrated value of $A$ is simply

$$\langle \Psi | A | \Psi \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T \langle \Psi | A(t) | \Psi \rangle dt = \sum_i |c_i|^2 A_{ii}. \quad (2)$$

The deviation of $A$ from equilibrium is captured by an auxiliary operator $\hat{A}$, that has the following form in the energy eigenbasis

$$\hat{A}_{ij} = \begin{cases} A_{ij}, & i \neq j \\ 0, & i = j \end{cases}. \quad (3)$$

We assume $A$ is bounded, $||A|| = 1$, thus without loss of generality $\hat{A}$ is bounded as well. Finally, we introduce time-dependent deviation from the equilibrium

$$a(t) := \langle \Psi | \hat{A}(t) | \Psi \rangle = \langle \Psi | A(t) | \Psi \rangle - \langle \Psi | A | \Psi \rangle = \sum_{i \neq j} c_i^* c_j A_{ij} e^{-i(E_i - E_j)t}.$$

(4)

The approach of $a(t)$ to zero can be explained from (4) through dephasing. The crucial question is to identify characteristic energy difference $\delta E \sim |E_i - E_j|$ which governs time dynamics. Clearly, $\delta E$ can not be larger than the energy variance of the initial state, but the latter is normally growing with the system size, which seemingly should result in vanishing equilibration times. It was suggested in [19] that $\delta E$ is bounded by the form of the matrix elements $A_{ij}$, which for local $A$ approach zero exponentially quickly for large $|E_i - E_j| \sim 1$. This can explain why characteristic equilibration timescales do not decrease for large system sizes, but fail to explain why they actually increase. To elucidate the approach of $a(t)$ to zero, we first consider a qualitative argument. We start with an initial out of equilibrium state $|1\rangle$ with large $\Delta E_\Psi$ and $a(0) \neq 0$ and consider
a(t) at some late time t. The initial state can be represented as a sum of $\Delta E_\Psi t/(2 \pi)$ states of the form \(|1\rangle\), each confined to its own interval of size $2\pi t$ centered at $E_k = E_\Psi + (2k - 1)\pi/t + \Delta E_\Psi$. $\Psi = \sum_{k=1}^{\Delta E_\Psi t/2\pi} \Psi_k$. Then qualitatively we can assume that different $\Psi_k$ are mutually dephased, such that

$$a(t) = \langle \Psi | \hat{A}(t) | \Psi \rangle \approx \sum_{k=1}^{\Delta E_\Psi t/2\pi} \langle \Psi_k | \hat{A}(t) | \Psi_k \rangle.$$  \hfill (5)

Each term in (5) is bounded in terms of the deviation functions $\hat{x}_{\max/\min}(E, \Delta E)$ which are defined as the maximal/minimal eigenvalues of matrix $\hat{A}_{ij}$ projected on the interval $[E - \Delta E, E + \Delta E]$. These functions are closely related to the deviation functions $x_{\max/\min}(E, \Delta E)$ introduced in [23] with the only difference being that in the latter case the corresponding matrix is $A_{ij}$. (In other words $\hat{x}$ and $x$ differ only by the inclusion of the diagonal elements $A_{ii}$ and in the quantum ergodic case functions $\hat{x}$ and $x$ are the same up to unimportant volume-suppressed corrections. In the integrable case these functions are different. A more detailed comparison of $x$ and $\hat{x}$ can be found in the Appendix.) Assuming functions $\hat{x}$ smoothly depend on the mean energy of the interval, all $E_k$ can be substituted by $E_\Psi$ and we find

$$\hat{x}_{\max}(E_\Psi, \pi/t) \geq a(t) \geq \hat{x}_{\min}(E_\Psi, \pi/t).$$  \hfill (6)

This bound can not uniformly apply to all states even at late times. We show in the Appendix that it is always possible to find an initial state such that different $\Psi_k$ become mutually coherent at any given point in time $t = t^*$ and both $a(0)$ and $a(t^*)$ are far from being zero. Nevertheless a similar bound applies to the time-averaged $a(t)$,

$$\langle a \rangle_T = \int_{-\infty}^{\infty} dt \frac{\sin(\pi t/T)}{\pi t} a(t).$$  \hfill (7)

The time average $\langle a \rangle_T$ can be bounded by the extreme eigenvalues $\hat{x}_{\max/\min}(E, \Delta E)$ of the band matrix $\hat{A}_{\Delta E}$,

$$\langle \hat{A}_{\Delta E} \rangle_{ij} = \begin{cases} \hat{A}_{ij}, & |E_i - E_j| \leq \Delta E, \\ 0, & |E_i - E_j| \geq \Delta E, \end{cases}$$

$$E_i, E_j \in [E - \Delta E, E + \Delta E].$$  \hfill (8)

To clarify, $\hat{x}$ stands for the extreme eigenvalues of matrix $\hat{A}_{ij}$ restricted to the interval \([1]\), while $\hat{x}$ stands for extreme eigenvalues of the same matrix after taking certain off-diagonal elements to be zero. The difference in definitions of $\hat{x}$ and $\hat{x}$ is visualized in Fig. 1. It was shown in \([23]\) in full generality that for any initial $\Psi$ and $T$

$$2\hat{x}_{\max}(E', \pi/T) + \hat{x}_{\max}(E'', \pi/(2T)) \geq \langle a \rangle_T,$$  \hfill (9)

and a similar inequality bounds $\langle a \rangle_T$ from below. Energies $E'$ and $E''$ have to belong to the original interval \([1]\) associated with $\Psi$. Assuming that $\hat{x}$ and $\hat{x}$ smoothly depend $E$ only through the effective temperature, so far

the original state has relatively small energy variance $\Delta E_\Psi \ll E_\Psi$ one can substitute $E', E''$ by $E_\Psi$.

A priori $\hat{x}$ and $\hat{x}$ are not directly related. The former quantity measures maximal deviation from the equilibrium $a(0)$ for all states of the form \(|1\rangle\) with $E_\Psi = E$ and $\Delta E_\Psi = \Delta E$, while the latter measures maximum value of $\langle a \rangle_x/\Delta E$ for the same class of initial states. In case $a(t)$ is oscillating exactly with the period $\pi/\Delta E$, $|\hat{x}|$ can be much larger than $|\hat{x}|$. At the same time for a wide class of systems we expect $a(t)$ not to exhibit persistent oscillations with the time periods equal to or exceeding the timescales associated with the macroscopic transport. Thus, for quantum ergodic systems, for which all off-diagonal matrix elements of local observables were verified to be exponentially small \([25]\), we expect that substituting certain matrix elements with zero can not parametrically increase extreme eigenvalues. Hence for sufficiently small $\Delta E$, we expect $\hat{x}$ can be bounded in terms of $\hat{x}$,

$$\hat{x}_{\max}(E, \Delta E) \leq \kappa \hat{x}_{\max}(E, \Delta E),$$

$$\hat{x}_{\min}(E, \Delta E) \geq \kappa \hat{x}_{\min}(E, \Delta E).$$  \hfill (10)

Here $\kappa$ is some constant, which is $\Delta E$ and system size-independent. This bound with different values of $\kappa$ may apply more generally e.g. to integrable systems, as we demonstrate numerically below. In all cases considered $\kappa \leq 1$. Using monotonicity of $\hat{x}$ as a function of $\Delta E$, we find that for sufficiently large $T$ (compare with \([6]\)),

$$\kappa' \hat{x}_{\max}(E_\Psi, \pi/T) \geq \langle a \rangle_T \geq \kappa' \hat{x}_{\min}(E_\Psi, \pi/T),$$  \hfill (11)

where $\kappa' \leq 3\kappa$ is some constant of order 1. This bound applies to all initial states with $\Delta E_\Psi \ll E_\Psi$ and for times $T$ not exceeding Heisenberg time.
Below we provide numerical evidence for (11,12) and (7). For large $T$ exceeding Thouless time the integral (7) can be approximated as (here we also assume $a(t)$ is an even function of $t$)

$$\langle a \rangle_T \approx 2 \int_0^\infty a(t)dt/T.$$  \hspace{1cm} (16)

Using late time approximation $a(t) \approx a(0)e^{-t/\tau_D}$ we find $\langle a \rangle_T \approx 2\tau_D/T$, where $\tau_D$ is the diffusive, or Thouless, time. Hence the slope of $\langle a \rangle_T$, as a function of $\Delta E = \pi/T$ can be associated with $\tau_D$. The plots in Fig. 2 demonstrate that $2\tau_D$ is approximately equal to $\tau$. Identifying $\tau$ as Thouless time provides the following interpretation: the inequalities (13) uniformly apply to all states for times $T$ equal to or exceeding timescales of macroscopic equilibration.

Remarkably the inequalities (13) with $\kappa' = 1$ are approximately saturated at $T \approx \tau/2$ by the square-wave configurations with largest amplitudes (see Fig. 2). The points of saturation approximately coincide with the points of largest curvature of $\Delta \hat{E}(x)$, $x_+$ and $x_-$. It can be also shown analytically that $\Delta \hat{E}(x) = \pm 1$ remains finite in the limit $L \to \infty$. Combining this with the monotonicity of $\hat{x}_{\text{max/min}}$ as a function of $\Delta E$ suggests the following behavior of $\Delta \hat{E}(x)$ in the thermodynamic limit. As $L$ increases $\Delta \hat{E}(x)$ will remain finite for $-1 \leq x < x_-$ and $x_+ < x \leq 1$ and will go to zero at least as $1/L^2$ for $x_+ \geq x \geq x_-$. Hence Thouless energy can be defined as the value of $\Delta \hat{E}(x)$ at the boundary points of the region $[x_-, x_+]$, within which $\Delta \hat{E}(x)$ approaches zero in the thermodynamic limit.

It is instructive to discuss the behavior of $\Delta \hat{E}(x)$ and $\Delta \hat{E}(x)$ at small $x$. It can be shown in full generality that for $\Delta E$ much smaller than the inverse macroscopic equilibration times

$$x^2 \geq \frac{\Delta Ef^2(0)}{4\pi},$$ \hspace{1cm} (17)

$$f^2(0) := \lim_{\omega \to 0} \int_{-\infty}^{\infty} dt e^{-i\omega t} \langle A(t)A(0) \rangle.$$ \hspace{1cm} (18)

The autocorrelation function in (18) is calculated over the microcanonical window $[E - \Delta \hat{E}/2, E + \Delta \hat{E}/2]$ (see Appendix for details). For most observables $f^2(0)$ remains finite or grows with the system size in the thermodynamic limit (for a diffusive quantity in 1D $f^2(0) \sim L$ (29, 30), although there are observables, e.g. the operators of the form $A = i[H, B]$, for which $f^2(0) = 0$. Such observables are excluded from further consideration. The inequal-

**FIG. 2.** Plots of $\Delta \hat{E}(E, x)$ (blue dotted line) and $\Delta \hat{E}(E, x)$ (yellow dashed line) for $A = \sigma_z^\ell$, $h = 0.7$. $L = 17$, $E = 0$, superimposed with the plots of $x = \langle a \rangle_T$ as a function of $\Delta E = \pi/T$ (black lines) for $\ell = 9$, $c_1 = -11.44$, $c_2 = 10.63$ (left) and $\ell = 9$, $c_1 = 12.02$, $c_2 = -14.46$ (right). Straight black dotted lines is the linear fit of $\langle a \rangle_T/\Delta E$ for small $\Delta E$. Their values at $x = \pm 1$ give the approximate value of $\pi/(2\tau_D) \approx 0.04$. Green squares in the background show $(5/L^2)x^2/\Delta E$ as a function of $\hat{x}$. The overall scaling coefficient $5/\Delta E$ is chosen by convenience to fit $x^2/\Delta E$ on the same plot with $\Delta \hat{E}(x)$.
ity [17] means that near the origin $\Delta \hat{E}(x)$, $\Delta \tilde{E}(x)$ grow slowly, not faster than a parabola. 

The bound [13] is approximately saturated at $T = T^*$ by the state $|\hat{\Psi}\rangle$ which maximizes the deviation $\langle \hat{\Psi} | \hat{A} | \hat{\Psi} \rangle$ for the given value of $\Delta E_{\Psi} = \pi/T^*$. We would call such states the “slowest.” For such states $a(0) = \tilde{x}(\Delta E_{\Psi})$ and $|\langle \hat{\Psi} | a(0) | \hat{\Psi} \rangle| \leq 2|a(0)| \Delta E_{\Psi}$, which gives $a(T) \approx \tilde{x}(\pi/T^*)$. If we define equilibration time for such states as the value of $T\langle a \rangle_T$ for very large $T$, it will be at least of the order $|a(0)|/\Delta E_{\Psi} \geq f(0)/\Delta E_{\Psi}^{1/2}$. By choosing $\Delta E_{\Psi}$ sufficiently small one can make equilibration time arbitrarily long. Thus, in full generality a diffusive system admits a family of states which remain out of equilibrium parametrically longer than Thouless time. It remains to be seen what role these states may play at the macroscopic level.

Finally, we discuss another characteristic of equilibration dynamics, the integrated expectation value variance

$$T = \int_0^{T^*} a(t)^2 \, dt.$$  \hspace{1cm} (19)

We estimate $T$ for the “slowest” states introduced above as the initial amplitude-squared $|a(0)|^2$ multiplied by the characteristic time $|a(0)|/|\tilde{a}| \sim T^* = \pi/\Delta E_{\Psi}$ necessary for $a(t)$ to approach zero. This gives

$$T \geq T_0(\Delta E_{\Psi}), \quad T_0 := \tilde{x}^2(\Delta E)/6\Delta E.$$  \hspace{1cm} (20)

In the ergodic case matrix $\hat{A}_{ij}$ inside a sufficiently small energy interval is expected to be random [24] causing [17] to be saturated up to a numerical factor. Hence, for small $\Delta E$, $T_0 \approx f^2(0) \sim L$. When $\Delta E$ becomes larger, of order of Thouless energy, $\tilde{x} \sim x_\pm \sim 1$ and $T_0 \approx \tau_D \sim L^2$. This is the largest value of $T_0$. For larger $\Delta E$, $T_0$ decreases and eventually goes to zero. This behavior, with two peak clear at $x \sim x_\pm$ is shown in Fig. 2 where we plot $x^2/\Delta \hat{E}(x)$ as a function of $x$. To summarize, for an ergodic quantum many-body system Thouless time can be defined as the maximal value of $x^2/\Delta E(x)$. It is also interesting to see if Thouless time can impose a universal upper bound on $T$ [19] for all initial states provided the ergodic system exhibits only one type of transport.

Next, we discuss the integrable case $h = 0$. The corresponding plots for $A = \sigma_x^1$ are shown in Fig. 3. First we notice that $\Delta \hat{E}(x) \leq \Delta \tilde{E}(x)$ for $\Delta E \leq \pi/\tau \approx 0.6$. The plots of $\langle a \rangle_T$ as a function of $T$ for macroscopic configurations reach their maximal values at $T \sim 2\tau$. This time can be identified as the ballistic time. Hence the inequality [13] is satisfied already for times somewhat smaller than the macroscopic equilibration timescales. The plot of $x^2/\Delta \hat{E}$ exhibits two peaks, as in the ergodic case, but in the integrable case we expect the value of the peaks to scale as $L$, consistent with the ballistic transport.

We note that $\langle a \rangle_T$ as a function of $\Delta E = \pi/T$ becoming larger than $\tilde{x}(\Delta E)$ and $\tilde{x}(\Delta E)$ is not a violation of [13], because of $\kappa'$. It is interesting that for small $\Delta E$, the behavior of $\langle a \rangle_T$ essentially coincides with $\tilde{x}(\Delta E)$. This could mean that for sufficiently late time [13] is satisfied with $\kappa' = 1$.

The behavior of $\Delta \hat{E}(x)$ at the origin implies that $f^2(0)$ for $A = \sigma_x^1$ vanishes. The same behavior is exhibited by some other, but not all, local operators. Following [31], we attribute this to the corresponding integrable system being non-interacting.

The operators $A = \sigma_z^1, A = \sum_{k=1}^L \sigma_z^k/L$, and $A = \sum_{k=1}^L \sigma_z^k/L$ are discussed in the Appendix. In all cases the expectation value in the state $\Psi$ projected on an energy interval of size $2\pi/T$. The longest macroscopic timescale is determined by the size of the smallest energy interval necessary to achieve a large deviation from the equilibrium. This picture is made precise by the bound [13], which constrains time-averaged expectation value in terms of the deviation functions $\tilde{x}_{\max/min}(\Delta E)$. We identified the longest macroscopic equilibration timescale (Thouless time in the diffusive case) as the maximal value of $x^2/\Delta \hat{E}(x)$, or, equivalently, the inverse value of $\Delta \hat{E}(x)$ at the boundary points $x_\pm$ of the interval, within which $\Delta \hat{E}(x)$ goes to zero in the thermodynamic limit.

Our results open several new research directions. A uniform bound that constrains the expectation value

![Fig. 3. Plots of $\Delta \hat{E}(E, x)$ (blue dotted line) and $\Delta \tilde{E}(E, x)$ (yellow dashed line) for $A = \sigma_x^1, h = 0, L = 17, E = 0$, superimposed with the plots of $x = \langle a \rangle_T$ as a function of $\Delta E = 2\pi/T$ (black lines) for $\ell = 9, e_1 = -11.45, e_2 = 10.14$ (left) and $\ell = 8, e_1 = 10.14, e_2 = -11.45$ (right). Green squares in the background show $(5/L)x^2/\Delta \hat{E}$ as a function of $\tilde{x}$. The overall scaling coefficient $5/L$ is chosen by convenience to fit $x^2/\Delta \hat{E}$ on the same plot with $\Delta \hat{E}(x)$.](image-url)
dynamics for all initial states is a potent result, and it would be important to understand if a similar bound applies more generally, beyond ergodic and non-interacting integrable systems. Another important question is to establish the bound analytically by outlining necessary conditions for the inequalities \[11,12\]. It is also likely that a similar bound will apply to other time-averaged quantities,

\[
\frac{1}{T} \int_0^T a(t) dt \quad \text{or} \quad \frac{1}{\pi^{1/2} T} \int_{-\infty}^{\infty} e^{-(t/T)^2} a(t) dt. \tag{21}
\]

Finally, for an ergodic many-body system the behavior of function \(\Delta E(x)\) provides a definition of Thouless time, as the time of macroscopic relaxation dynamics. It would be important to relate this definition to other notions based on the amplitude of matrix elements \([29,32]\) or spectral properties \([33]\).

**Acknowledgments.** I am grateful to Joel Lebowitz and David Huse for helpful discussions. I would also like to thank Tomaz Prosen, Hong Liu, Moshe Rozali, and Luis Pedro Garcia-Pintos for reading the manuscript and helpful comments. I acknowledge the University of Kentucky Center for Computational Sciences for computing time on the Lipscomb High Performance Computing Cluster.

**APPENDIX**

**States that deviate from equilibrium at \(t = 0\) and any given moment of time \(t = t^*\)**

We would like to show that there are always special states \(\Psi\) which are out-of-equilibrium at the initial moment of time \(t = 0\) and at any given moment \(t^*\). We first show that heuristically and then give a rigorous argument in the Theorem 1 below.

Let us start with an out-of-equilibrium state \(\Psi_0\) such that \(a_0 = \langle \Psi_0|A|\Psi_0\rangle \neq 0\). We consider

\[
\Psi = \frac{\Psi_0(0) + \Psi_0(-t^*)}{\sqrt{2}}, \tag{22}
\]

where \(\Psi_0(t)\) stands for the time-evolved state in the Schrödinger picture. Then \((22)\) is out-of-equilibrium both as \(t = 0\) and \(t = t^*\), with \(a(0) = a_0/2\) and \(a(t^*) = a_0/2\). Here we assumed that \(t^*\) is large enough such that \(\Psi_0\) and \(\Psi_0(t^*)\) are sufficiently dephased and \(\langle \Psi_0|\Psi_0(t^*)\rangle \approx \langle \Psi_0|A|\Psi_0(t^*)\rangle \approx 0\). The following theorem makes these additional assumptions unnecessary.

**Theorem 1.** Let \(a_{\text{max}}\) and \(a_{\text{min}}\) be the largest and smallest eigenvalues of matrix \(A\). Then in full generality for any given time \(t^*\) there is an initial state \(\Psi\) such that

\[
a(0) \geq \frac{3a_{\text{max}} + a_{\text{min}}}{4} \quad \text{or} \quad a(0) \leq \frac{3a_{\text{min}} + a_{\text{max}}}{4}, \tag{23}
\]

and

\[
a(t^*) \geq \frac{3a_{\text{max}} + a_{\text{min}}}{4} \quad \text{or} \quad a(t^*) \leq \frac{3a_{\text{min}} + a_{\text{max}}}{4}. \tag{24}
\]

**Proof.** We would like to consider a set of points

\[
F = \{(a(0), a(t^*)) | |\Psi| = 1\}. \tag{25}
\]

defined for all normalized vectors \(\Psi\). \(F\) is a compact set which is fully contained within a square region specified by inequalities \(a_{\text{max}} \geq a(0) \geq a_{\text{min}}\) and \(a_{\text{max}} \geq a(t^*) \geq a_{\text{min}}\). There are points in \(F\) which saturate each of these four inequalities (we denote them \(a,b,c,d\) in Fig. 4). By definition, the set \(F\) is a joint numerical range of matrices \(\hat{A}(0)\) and \(\hat{A}(t^*)\) (in Heisenberg picture). The Toeplitz-Hausdorff theorem \([34,36]\) assures that \(F\) is convex. From here it follows that one of the points

\[
A = \frac{(3a_{\text{max}} + a_{\text{min}},3a_{\text{max}} + a_{\text{min}})}{4}, \tag{26}
\]

\[
B = \frac{(3a_{\text{max}} + a_{\text{min}},3a_{\text{min}} + a_{\text{max}})}{4}, \tag{27}
\]

\[
C = \frac{(3a_{\text{min}} + a_{\text{max}},3a_{\text{max}} + a_{\text{min}})}{4}, \tag{28}
\]

\[
D = \frac{(3a_{\text{min}} + a_{\text{max}},3a_{\text{min}} + a_{\text{max}})}{4}, \tag{29}
\]

belongs to \(F\). This finishes the proof. As a comment, we notice that this theorem can be formulated for the states of the form \([11]\) with any \(E, \Delta E\). Then \(a_{\text{max}}\) and \(a_{\text{min}}\) would be the maximal and minimal eigenvalues of \(\hat{A}\) projected on the corresponding subspace of the full Hilbert space. Since any projection of \(\hat{A}\) is traceless, \(a_{\text{max}} > 0\) and \(a_{\text{min}} < 0\) for all \(E, \Delta E\).

The meaning of this theorem is simple: there is always an initial state \(\Psi\) which is out of equilibrium at the initial moment of time \(t = 0\) and at any given moment of time \(t = t^*\). The universal nature of this result applicable for all quantum systems does not necessarily allow the deviation at the given moment of time \(a(t^*)\) to be of the same sign as \(a(0)\). Indeed, one can consider a harmonic oscillator with the period \(T = 2\pi\). Then, independently of the initial conditions \(a(\pi) = -a(0)\) where \(a(t)\) is the coordinate of the oscillator.

**Relation between \(\Delta E(x), \Delta \hat{E}(x)\), and connection to canonical universality**

In \([23]\) we have introduced \(x_{\text{max/min}}(E,\Delta E)\) as the maximal/minimal eigenvalue of an observable \(A\) projected on an energy interval \([E - \Delta E, E + \Delta E]\), after subtracting microcanonical expectation value of \(\hat{A}\),

\[
x_{\text{max/min}} = \lambda_{\text{max/min}}(A_{ij}) - \langle A \rangle_E, \tag{30}
\]

\[
\langle A \rangle = \frac{1}{N} \sum_i A_{ii}. \tag{31}
\]
FIG. 4. Points $a, b, c, d$ which saturate inequalities $a_{\text{max}} \geq a(0) \geq a_{\text{min}}$ and $a_{\text{max}} \geq a(t^*) \geq a_{\text{min}}$. Joint numerical range $F$ is convex and therefore includes gray polygon area formed by these four points. Consequently $F$ includes at least one of the four points $A, B, C, D$ highlighted in red. Indeed the only polygon region which does not include $A, B, C, D$ as internal points (although it includes all of them as the boundary points) and touches the boundaries $a(0) = a_{\text{max}}, a(0) = a_{\text{min}}, a(t^*) = a_{\text{max}}, a(t^*) = a_{\text{min}}$ is the blue dotted square formed by the points $a', b', c', d'$. Any attempt to move points $a', b', c', d'$ along the boundaries will make at least one of the points $A, B, C, D$ to be inside $F$.

Here by $N(\Delta E)$ the total number of energy states inside the interval $[E - \Delta E, E + \Delta E]$, and $\lambda_{\text{max/min}}(X)$ stands for the largest/smallest eigenvalue of a Hermitian matrix $X$. In this paper we introduced $\hat{x}_{\text{max/min}}(E, \Delta E)$ of an observable $\hat{A}$ projected on an energy interval $[E - \Delta E, E + \Delta E]$, after taking all diagonal matrix elements to be zero,

$$\hat{x}_{\text{max/min}} = \lambda_{\text{max/min}}(\hat{A}_{ij}).$$

Clearly both definitions are closely related. Thus, in the quantum ergodic case when the observables $A_{ij}$ satisfied the Eigenstate Thermalization Hypothesis ansatz both functions coincide up to unimportant volume-suppressed corrections. Indeed, matrix $A_{ij}$ can be represented as a sum $A_{ij} = \hat{A}_{ij} + D_{ij}$, where $D_{ij} = \delta_{ij} \delta_{ij}$. Using the triangle inequality we can find

$$|x - \hat{x}| \leq |D_{ij} - \langle A \rangle E \delta_{ij}|.$$  

(33)

The matrix $D_{ij} - \langle A \rangle E \delta_{ij}$ is diagonal and its norm is equal to the value of the largest diagonal element, which can be easily estimated to be $\Delta E / \text{Volume small}$. Comparing with the behavior $x(\Delta E) \geq f(0) \Delta E^{1/2}$ (see section below), we conclude that the contribution of the diagonal elements in the ergodic case is negligible. Instead of dealing with the functions $\hat{x}_{\text{max}}$ and $\hat{x}_{\text{min}}$ and similarly $x_{\text{max/min}}$ it is convenient to introduce single-valued inverse functions $\Delta E(x)$ and $\hat{\Delta} E(x)$. In the ergodic case both functions are smooth and become zero only at $x = 0$, a property dubbed canonical universality in [23]. This is illustrated in Fig. 5.

In the integrable case the behavior of $\Delta E(x)$ and $\hat{\Delta} E(x)$ are different as the contribution of the diagonal matrix elements is not negligible. Both functions are only piece-wise continuous, see Figure 3 and Figure 7 below.

**Behavior of $\Delta E(x)$ at small $x$**

For any $N \times N$ Hermitian matrix $A_{ij}$ maximal (by absolute value) eigenvalue $\hat{x}$ is bounded by $N\hat{x}^2 \geq \text{Tr} AA^\dagger = \sum_{i,j} |A_{ij}|^2$. Let us consider a projection of the full matrix $\hat{A}_{ij}$ of an observable $\hat{A}$ on the energy interval $[E - \Delta E, E + \Delta E]$. By $N(\Delta E)$ we denote the total num-

![Graph](image-url)
Let us introduce an autocorrelator of $A$ defined as an average over the microcanonical window $[E - \Delta E, E + \Delta E]$,
\[
\langle A(t)A(0) \rangle_{\Delta E} = \frac{1}{N(\Delta E)} \sum_{i,j} |\langle A_{ij} \rangle|^2, \quad E_i, E_j \in [E - \Delta E, E + \Delta E].
\]

The second term in the parenthesis ensures that $\langle A(t)A(0) \rangle_{\Delta E}$ approaches zero at late time $t$. Then
\[
\hat{x}(\Delta E)^2 \geq \frac{N(\Delta E/2)}{\pi N(\Delta E)} \int_{-\infty}^{\infty} dt \sin(t\Delta E/2) \langle A(t)A(0) \rangle_{\Delta E/2},
\]
where we substituted the sum in (34) by a partial sum over the matrix elements shown in the gray area in Fig. 6.

Assuming $\Delta E$ is substantially small such that the density of states $\Omega(E)$ is almost constant within the interval, $N(\Delta E/2)/N(\Delta E) \sim 1/2$, and we find
\[
\hat{x}(\Delta E)^2 \geq \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \sin(t\Delta E/2) \langle A(t)A(0) \rangle_{\Delta E/2}.
\]

For a many-body quantum system the autocorrelation function $\langle A(t)A(0) \rangle_{\Delta E/2}$ will not depend on the size of the microcanonical window provided it includes exponentially many states, $\Delta E \gg \Omega^{-1}$. This puts the bound on how small $\Delta E$ we can consider. When $\Delta E$ is much smaller than the inverse timescale associated with saturation of $\langle A(t)A(0) \rangle$ (normally it would remain finite or grow polynomially with the system size), the integral in (36) can be approximated as
\[
\int_{-\infty}^{\infty} dt \sin(t\Delta E/2) \langle A(t)A(0) \rangle_{\Delta E/2} \approx \frac{\Delta E f^2(0)}{4\pi},
\]
but the same inequality also applies to $\Delta E(x)$ and $\Delta E(x)$.

The latter integral approaches a constant or grows polynomially with the system size for most observables. Here we define $f^2(0)$ via (38), but for the quantum ergodic systems satisfying the ETH [29] function $f(\omega)$ has an independent meaning. In the latter case the bound (36) can be somewhat improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The inequality (37) can be conveniently rewritten as
\[
\Delta E(x) \leq \frac{4\pi x^2}{f^2(0)},
\]
and Figure 8 shows how the bound in (36) can be improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The latter integral approaches a constant or grows polynomially with the system size for most observables. Here we define $f^2(0)$ via (38), but for the quantum ergodic systems satisfying the ETH [29] function $f(\omega)$ has an independent meaning. In the latter case the bound (36) can be somewhat improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The inequality (37) can be conveniently rewritten as
\[
\Delta E(x) \leq \frac{4\pi x^2}{f^2(0)},
\]
and Figure 8 shows how the bound in (36) can be improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The latter integral approaches a constant or grows polynomially with the system size for most observables. Here we define $f^2(0)$ via (38), but for the quantum ergodic systems satisfying the ETH [29] function $f(\omega)$ has an independent meaning. In the latter case the bound (36) can be somewhat improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The inequality (37) can be conveniently rewritten as
\[
\Delta E(x) \leq \frac{4\pi x^2}{f^2(0)},
\]
and Figure 8 shows how the bound in (36) can be improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The latter integral approaches a constant or grows polynomially with the system size for most observables. Here we define $f^2(0)$ via (38), but for the quantum ergodic systems satisfying the ETH [29] function $f(\omega)$ has an independent meaning. In the latter case the bound (36) can be somewhat improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The inequality (37) can be conveniently rewritten as
\[
\Delta E(x) \leq \frac{4\pi x^2}{f^2(0)},
\]
and Figure 8 shows how the bound in (36) can be improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The latter integral approaches a constant or grows polynomially with the system size for most observables. Here we define $f^2(0)$ via (38), but for the quantum ergodic systems satisfying the ETH [29] function $f(\omega)$ has an independent meaning. In the latter case the bound (36) can be somewhat improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.

The inequality (37) can be conveniently rewritten as
\[
\Delta E(x) \leq \frac{4\pi x^2}{f^2(0)},
\]
and Figure 8 shows how the bound in (36) can be improved by expressing the full sum from (34) in terms of $f^2(\omega)$. We refer the reader to [23] for details, including the numerical plots of $\sum_{i,j} |A_{ij}|^2/N^2$ as a function of $\Delta E$ in case of a non-integrable spin chain.
[2] Sandu Popescu, Anthony J Short, and Andreas Winter, “Entanglement and the foundations of statistical mechanics,” Nature Physics 2, 754 (2006).
[3] Peter Reimann, “Typicality for generalized microcanonical ensembles,” Physical review letters 99, 160404 (2007).
[4] Peter Reimann, “Foundation of statistical mechanics under experimentally realistic conditions,” Physical Review Letters 101, 190403 (2008).
[5] Noah Linden, Sandu Popescu, Anthony J Short, and Andreas Winter, “Quantum mechanical evolution towards thermal equilibrium,” Physical Review E 79, 061103 (2009).
[6] Sheldon Goldstein, Joel L Lebowitz, Roderich Tumulka, and Nino Zanghì, “Long-time behavior of macroscopic quantum systems,” The European Physical Journal H 35, 173–200 (2010).
[7] Noah Linden, Sandu Popescu, Anthony J Short, and Andreas Winter, “On the speed of fluctuations around thermodynamic equilibrium,” New Journal of Physics 12, 055021 (2010).
[8] Anthony J Short, “Equilibration of quantum systems and subsystems,” New Journal of Physics 13, 053009 (2011).
[9] Peter Reimann, “Equilibration of isolated macroscopic quantum systems under experimentally realistic conditions,” Physica Scripta 86, 058512 (2012).
[10] Peter Reimann, “Generalization of von neumanns approach to thermalization,” Physical review letters 115, 010403 (2015).
[11] Christian Gogolin and Jens Eisert, “Equilibration, thermalisation, and the emergence of statistical mechanics in closed quantum systems,” Reports on Progress in Physics 79, 056001 (2016).
[12] H Wilming, TR de Oliveira, AJ Short, and J Eisert, “Equilibration times in closed quantum many-body systems,” arXiv preprint arXiv:1805.06422 (2018).
[13] Anthony J Short and Terence C Farrelly, “Quantum equilibration in finite time,” New Journal of Physics 14, 013063 (2012).
[14] Artur SL Malabarba, Luis Pedro García-Pintos, Noah Linden, Terence C Farrelly, and Anthony J Short, “Quantum systems equilibrate rapidly for most observables,” Physical Review E 90, 012121 (2014).
[15] S Goldstein, T Hara, and H Tasaki, “The approach to equilibrium in a macroscopic quantum system for a typical nonequilibrium subspace, preprint (2014),” arXiv preprint arXiv:1402.3380.
[16] Sheldon Goldstein, Takashi Hara, and Hal Tasaki, “Extremely quick thermalization in a macroscopic quantum system for a typical nonequilibrium subspace,” New Journal of Physics 17, 045002 (2015).
[17] Peter Reimann, “Typical fast thermalization processes in closed many-body systems,” Nature communications 7, 10821 (2016).
[18] Ben N Balz and Peter Reimann, “Typical relaxation of isolated many-body systems which do not thermalize,” Physical review letters 118, 190601 (2017).
[19] Th mango R de Oliveira, Christos Charalambous, Daniel Jonathan, Maciej Lewenstein, and Arnau Riera, “Equilibration time scales in closed many-body quantum systems,” New Journal of Physics 20, 033032 (2018).
[20] M Cramer, “Thermalization under randomized local hamiltonians,” New Journal of Physics 14, 053051 (2012).
[21] Luis Pedro García-Pintos, Noah Linden, Artur SL Malabarba, Anthony J Short, and Andreas Winter, “Equilibration time scales of physically relevant observables,” Physical Review X 7, 031027 (2017).
[22] Sheldon Goldstein, Takashi Hara, and Hal Tasaki, “Time scales in the approach to equilibrium of macroscopic quantum systems,” Physical review letters 111, 140401 (2013).
[23] Anatoly Dymarsky and Hong Liu, “Canonical universality,” arXiv preprint arXiv:1702.07722 (2017).
[24] Anatoly Dymarsky, “Bound on eigenstate thermalization from transport,” arXiv preprint arXiv:1804.08626 (2018).
[25] Anatoly Dymarsky, Nima Lashkari, and Hong Liu, “Subsystem eigenstate thermalization hypothesis,” Physical Review E 97, 012140 (2018).
[26] Hu yuong Kim and David A Huse, “Ballistic spreading of entanglement in a diffusive nonintegrable system,” Physical review letters 111, 127205 (2013).
[27] V Kerala Varma, Alessio Lerose, Francesca Pietracaprina, John Goold, and Antonello Scardicchio, “Energy diffusion in the ergodic phase of a many body localizable spin chain,” Journal of Statistical Mechanics: Theory and Experiment 2017, 053101 (2017).
[28] Anatoly Dymarsky, “to appear,” .
[29] Luca D’Alessio, Yariv Kafri, Anatoli Polkovnikov, and Marcos Rigol, “From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics,” Advances in Physics 65, 239–362 (2016).
[30] David J Luitz and Yevgeny Bar Lev, “Anomalous thermalization in ergodic systems,” Physical review letters 117, 170404 (2016).
[31] Herbert Spohn, “Interacting and noninteracting integrable systems,” arXiv preprint arXiv:1707.02159 (2017).
[32] Maksym Serbyn, Z Papić, and Dmitry A Abanin, “Thouless energy and multifractality across the many-body localization transition,” Physical Review B 96, 104201 (2017).
[33] Amos Chan, Andrea De Luca, and JT Chalker, “Spectral statistics in spatially extended chaotic quantum many-body systems,” arXiv preprint arXiv:1803.03841 (2018).
[34] Otto Toeplitz, “Das algebraische analogon zu einem satze von fejér,” Mathematische Zeitschrift 2, 187–197 (1918).
[35] Felix Hausdorff, “Der wertvorrat einer bilinearform,” Mathematische Zeitschrift 3, 314–316 (1919).
[36] Karl Gustafson, “The toeplitz-hausdorff theorem for linear operators,” Proceedings of the American Mathematical Society 25, 203–204 (1970).