Bound on Eigenstate Thermalization from Transport

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(Received 4 May 2018; revised 8 October 2021; accepted 25 April 2022; published 11 May 2022)

We show that macroscopic thermalization and transport impose constraints on matrix elements entering the eigenstate thermalization hypothesis (ETH) ansatz and require them to be correlated. It is often assumed that the ETH reduces to random matrix theory (RMT) below the Thouless energy scale. We show that this conventional picture is not self-consistent. We prove that the energy scale at which the RMT behavior emerges has to be parametrically smaller than the inverse timescale of the slowest thermalization mode coupled to the operator of interest. We argue that the timescale marking the onset of the RMT behavior is the same timescale at which the hydrodynamic description of transport breaks down.

DOI: 10.1103/PhysRevLett.128.190601

Thermalization of isolated quantum systems has attracted significant attention recently. For quantum ergodic systems without local integrals of motion, it is currently accepted that thermalization can be explained with the help of the eigenstate thermalization hypothesis (ETH) [1–8]. At the technical level, the ETH can be understood as an ansatz for the matrix elements of observables in the energy eigenbasis [5]:

$$A_{ij} = A^{\text{eth}}(E)\delta_{ij} + \Omega^{-1/2}(E) f(E,\omega) r_{ij},$$
$$E = (E_i + E_j)/2, \qquad \omega = E_i - E_j. \tag{1}$$

Here, A is an observable satisfying ETH (1), $\Omega(E)dE$ is the density of states, A^{eth} and f are smooth functions of their arguments, and r_{ij} are pseudorandom fluctuations with unit variance. The diagonal part of the ETH ansatz explains thermalization, at least in the sense that the expectation value of A in some initial state with mean energy E, after averaging over time, is equal to the thermal expectation value of A at the effective temperature $\beta^{-1}(E) = d\ln\Omega/dE$. The dynamics of thermalization is encoded in the off-diagonal matrix elements r_{ij}, as well as in the initial state Ψ, and is not universal. In this Letter, we show that macroscopic thermalization, in particular, the type of transport present in the system, imposes constraints on the correlations of r_{ij}.

Numerical studies confirm that the r_{ij} behave "randomly" and oscillate around zero mean seemingly without any obvious pattern. Certainly, the r_{ij} cannot be random in the literal sense, as the form of A_{ij} is fixed once the Hamiltonian and A are specified. Moreover, A often has to satisfy various algebraic relations. For example, in a spin lattice model, one can choose A to be a Pauli matrix acting on a particular site. In this case, $A^2 = \mathbb{I}$, which requires r_{ij} to be correlated. Similarly, the r_{ij} can be constrained by the expected behavior of the four-point correlation function [9–12], etc.

While the whole matrix r_{ij} cannot be random, there is a strong expectation that fluctuations r_{ij} can be treated as random if the indexes i and j are restricted to belong to a sufficiently narrow energy interval. Assuming the interval is centered around some E, we define ΔE_{RMT} as the largest possible interval such that all r_{ij} with

$$|E_i - E|, |E_j - E| \le \Delta E_{\text{RMT}}/2 \tag{2}$$

can be treated for physical purposes as being random and independent (without necessary being normally distributed). The expectation that r_{ij} reduces to a Gaussian random matrix inside a sufficiently narrow interval is consistent with numerical studies which confirm that the r_{ij} are normally distributed [13–15] and that the form factor f becomes constant for ω smaller than inverse thermalization timescale $2\pi/\tau$, called the Thouless energy [16–19]. [Thouless energy ΔE_{Th} is often defined as a scale of applicability of RMT to describe statistics of the energy spectrum. Thermalization time τ is defined as the time when the autocorrelation function of an operator A approximately saturates to a constant. The inverse scale $2\pi/\tau$ is the size of the "plateau" of $f^2(\omega)$ and is also called Thouless energy in the literature. For certain systems and operators probing the slowest thermalization mode, both quantities are known to coincide $\Delta E_{\text{Th}} \approx 2\pi/\tau$ [19–21].] Furthermore, for real symmetric A_{ij}, the variances of the diagonal and off-diagonal elements have been numerically shown to satisfy $\langle r_{ii}^2\rangle = 2\langle r_{ij}^2\rangle$ [22–24], which is consistent with and necessary for r_{ij} to become a Gaussian orthogonal ensemble. Random behavior of r_{ij} also naturally emerges in the recent attempt to justify the ETH analytically [25]. From the physical point of view, the "structureless" form of

A_{ij} inside a small energy interval is expected on the grounds of the hypothetical universal behavior of observables at late times [26–33].

Reduction of r_{ij} to an RMT below $2\pi/\tau$ is seemingly in agreement with the conventional picture of thermalization. Assuming τ is the characteristic time of the slowest transport mode probed by A, after the time $t \gtrsim \tau$ the system will be in the ergodic regime; i.e., the value of A will not be sensitive to the initial state. This suggests r_{ij} should become structureless for $\Delta E_{\rm RMT} \sim 2\pi/\tau$ [18,19]. In this Letter, we show this is not the case, and $\Delta E_{\rm RMT}$ has to be *parametrically* smaller than the Thouless energy $2\pi/\tau$.

The key observation is that the ETH ansatz (1) with random mutually independent r_{ij} is constrained by the presence of states with extensively long thermalization times. Let us consider an initial state $|\Psi\rangle$, which describes an out-of-equilibrium configuration with an order one overlap with the slowest mode probed by A. Then, at late times

$$\delta A(t,\Psi) \sim e^{-t/\tau}, \quad t \gtrsim \tau, \tag{3}$$

where

$$\delta A(t,\Psi) = \langle\Psi|A(t)|\Psi\rangle - \sum_i |C_i|^2 A^{\rm eth}(E_i). \tag{4}$$

Here, the second term is simply the equilibrated value of A, such that δA asymptotes to zero at late times. We also assume $|\Psi\rangle$ has less than extensive energy variance ΔE. While our argument is more general, for concreteness one can think of a 1D spin chain of length L exhibiting diffusive transport of energy, and A would be a local operator coupled to energy. In this case, the initial state can be taken to describe a quasiclassical configuration with an extensive displacement of energy, while the timescale in Eq. (3) would be diffusive time $\tau \approx L^2/D$. An explicit construction of such a state $|\Psi\rangle$ is given in Supplemental Material [34].

To connect thermalization time τ to matrix elements of A, we introduce a parameter-dependent average, which is somewhat similar to the "average distance" used in Ref. [35]:

$$\langle\delta A\rangle_T \equiv \int_{-\infty}^{\infty} \delta A(t,\Psi) \frac{\sin(2\pi t/T)}{\pi t} dt. \tag{5}$$

Here, T is a free parameter. When T becomes large, Eq. (5) reduced to the conventional average over time T. After representing $A(t)$ in the energy eigenbasis using Eq. (1) and performing the integral in Eq. (5), we find

$$\langle\delta A\rangle_T = \langle\Psi|\delta A_T|\Psi\rangle, \tag{6}$$

where the operator δA_T written in the energy eigenbasis has the form

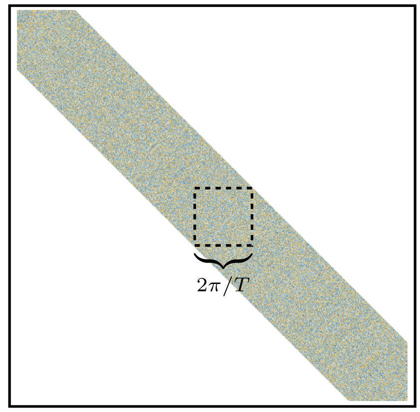

FIG. 1. Visualization of the band matrix $(\delta A_T)_{ij}$ (7).

$$(\delta A_T)_{ij} = \begin{cases} \Omega^{-1/2}(E) f(E,\omega) r_{ij}, & |E_i - E_j| \leq 2\pi/T, \\ 0, & |E_i - E_j| > 2\pi/T. \end{cases} \tag{7}$$

In other words, the matrix $(\delta A_T)_{ij}$ has a band structure, and it coincides with A_{ij} (after subtracting the nonrandom diagonal part) inside a diagonal band of size $2\pi/T$ and is zero outside. This is schematically shown in Fig. 1.

The expectation value $\langle\Psi|\delta A_T|\Psi\rangle$ can be bounded by the largest eigenvalue of δA_T, which we denote by $x(T)$:

$$|\langle\Psi|\delta A_T|\Psi\rangle| \leq x(T). \tag{8}$$

Let us assume now that T is sufficiently large such that $2\pi/T \leq \Delta E_{\rm RMT}$. Then, $(\delta A_T)_{ij}$ is a band random matrix with independent matrix elements, and its largest eigenvalue is controlled by the variance function $\overline{(\delta A_T)_{ij}^2} = \Omega^{-1} f^2(\omega)$ [36]. In the limit of a narrow band $T\Delta E \gg 1$ (see Supplemental Material [34]),

$$x^2(T) = 8 \int_0^{2\pi/T} f^2(E,\omega) d\omega. \tag{9}$$

Technically, Eq. (9) assumes the absence of correlations, while the definition of $\Delta E_{\rm RMT}$ (2) does not exclude possible correlations of r_{ij} and $r_{i'j'}$ along the diagonal, i.e., when $(E_i + E_j) - (E_i' + E_j')$ is large while $|E_i - E_j|$ and $|E_{i'} - E_{j'}|$ are small. In Supplemental Material [34], we justify Eq. (9) rigorously, using the result of Ref. [22], by converting it into an inequality. Looking ahead, our main result, inequality (11), continues to hold with different numerical coefficients.

With help of Eq. (1), the integral in the right-hand-side of Eq. (9) can be expressed through the connected autocorrelation function of A calculated at the effective inverse temperature $\beta^{-1} = d\ln\Omega/dE$ [16,17,19]:

$$\langle A(t)A(0)\rangle_\beta \equiv \langle E|A(t)A(0)|E\rangle - \langle E|A(0)|E\rangle^2. \tag{10}$$

Now, combining Eq. (8) with Eq. (9) written with help of Eq. (10), we find the inequality, which should be satisfied so far as $T \geq T_{\mathrm{RMT}} \equiv 2\pi/\Delta E_{\mathrm{RMT}}$:

$$|\langle\Psi|\delta A_T|\Psi\rangle|^2 = \left|\int_{-\infty}^{\infty} \delta A(t,\Psi)\frac{\sin(2\pi t/T)}{\pi t}dt\right|^2 \leq x^2(T)$$
$$= 4\int_{-\infty}^{\infty}\langle A(t)A(0)\rangle_\beta \frac{\sin(2\pi t/T)}{\pi t}dt. \quad (11)$$

The inequality (11) is our main technical result, which implies strong limitations on ΔE_{RMT}. As the characteristic size L of the system grows, the autocorrelation function of A approaches its thermodynamic form, which follows from the quasiclassical hydrodynamic description:

$$\langle A(t)A(0)\rangle_\beta \sim (t_D/t)^\alpha \quad (12)$$

with some L-independent $\alpha > 0$ and t_D. Coefficient α depends on the type of transport A couples to. The behavior (12) applies for $t \gtrsim t_D$ and persists until $t \approx \tau$, after which the autocorrelation function becomes zero [17,19]. Around the time $t \approx \tau$, the value of the full autocorrelation function, i.e., without the asymptotic value subtracted, should be inverse proportional to the volume, indicating that the conserved quantity coupled to A has spread across the whole system:

$$\left(\frac{t_D}{\tau}\right)^\alpha \propto \frac{1}{L^d}. \quad (13)$$

Here, L is a characteristic size of the system in dimensional units, e.g., the number of spins, while d is the number of spatial dimensions. Using Eq. (12) and for $T \gg t_D$, the right-hand side of Eq. (11) can be approximated as follows, where we dropped all numerical coefficients:

$$\int_0^\infty \langle A(t)A(0)\rangle_\beta \frac{\sin(2\pi t/T)}{\pi t}dt$$
$$\sim \begin{cases} (t_D/T)^\alpha, & \tau \gtrsim T \gg t_D, \\ (t_D/\tau)^\alpha \tau/T, & T \gtrsim \tau. \end{cases} \quad (14)$$

For late times $T \gg t_D$, Eq. (14) is very small irrespective of the value of τ/T. Strictly speaking, the estimate above is correct only as far as $\alpha < 1$ such that the integral gets its main contribution for large t. In most cases, this requires $d = 1$.

The behavior of the left-hand side of Eq. (11) is quite different. Starting from the exponential decay (3), we find, for large $T \gg \tau$,

$$\int_0^\infty \delta A(t,\Psi)\frac{\sin(2\pi t/T)}{\pi t}dt \sim \frac{\tau}{T}, \quad (15)$$

which is in agreement with the qualitative picture that $\delta A(t,\Psi)$ remains of the order of one for the time $t \sim \tau$ and then quickly approaches zero. When T is large but not necessarily larger than τ, Eq. (15) remains of the order of one and the inequality (11) cannot be satisfied. For Eq. (11) to be satisfied, T has to be parametrically larger than τ:

$$\left(\frac{\tau}{T}\right)^2 \lesssim \left(\frac{t_D}{\tau}\right)^\alpha \frac{\tau}{T} \Rightarrow T_{\mathrm{RMT}} \gtrsim \tau L^d. \quad (16)$$

In summary, we see that the inequality (11) imposes a stringent bound on the energy scale $\Delta E_{\mathrm{RMT}} = 2\pi/T_{\mathrm{RMT}}$, which should be *parametrically* smaller than the Thouless energy $2\pi/\tau$. In particular, for a 1D diffusive system and a local operator A coupled to a conserved quantity, we find

$$T_{\mathrm{RMT}} \gtrsim \tau L \sim L^3. \quad (17)$$

More generally, for any 1D system with local interactions, transport cannot be faster than ballistic, $\tau \propto L$, and, therefore, for any local operator, $T_{\mathrm{RMT}} \gtrsim \tau L \sim L^2$.

We illustrate the inequality (11) and the resulting difference between ΔE_{RMT} and τ^{-1} with the help of an open nonintegrable 1D Ising spin chain with two polarizations of the magnetic field. The operator $A = \sigma_x^1$ is a one-site operator. This model is diffusive. In Supplemental Material [34], where all technical details can be found, we numerically justify Eq. (3) as well as Eq. (12) with $\alpha = 1/2$. The result, the left-hand side and the right-hand side of Eq. (11), is shown in Fig. 2. The inequality is saturated for times T significantly larger than thermalization time τ, when the autocorrelation function plateaus (see the inset). This confirms the conclusion that the RMT timescale T_{RMT} is much larger than the thermalization time. The smallness of $\tau/T_{\mathrm{RMT}} \ll 1$ was also recently confirmed numerically in Refs. [24,37].

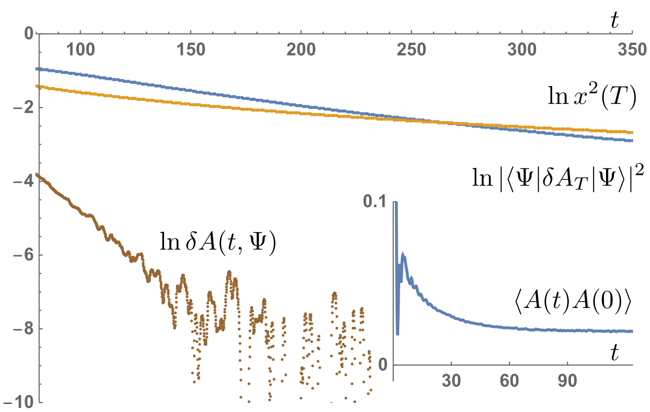

FIG. 2. Plots of the lhs and the rhs of Eq. (11) in logarithmic scale: $\ln|\langle\Psi|\delta A_T|\Psi\rangle|^2$ (blue lines) and $\ln x^2(T)$ (orange lines). Also shown in brown is $\ln \delta A(t,\Psi)$. Its approximately linear form (before saturation) confirms exponential decay (3). Inset: plot of the autocorrelation function. All plots are for a nonintegrable Ising spin chain with $L = 24$ spins with open bc; see Supplemental Material [34] for details.

For a translationally invariant system, it is also interesting to consider an operator A_k with a constant momentum. Keeping in mind a 1D diffusive spin lattice system of length L, we denote by $A_{(m)}$ a local operator A located at the site m. Then,

$$A_k = \frac{2^{1/2}}{L^{1/2}} \sum_{m=1}^{L} \cos(km) A_{(m)}, \tag{18}$$

where L is dimensionless. The normalization factor $(2/L)^{1/2}$ is chosen such that the connected autocorrelation function is L independent in the thermodynamic limit

$$\langle A_k(t) A_{-k} \rangle_\beta \simeq e^{-t/\tau_k}, \qquad \tau_k \propto k^2/D. \tag{19}$$

With the same normalization, the expectation value (4) in the state with a macroscopic amount of energy displaced will be

$$\delta A(t, \Psi) \sim L^{1/2} e^{-t/\tau_k}. \tag{20}$$

Although the t dependence in Eqs. (19) and (20) is the same, a different L-dependent prefactor will result in a constraint for T_{RMT}. For large $T \gg \tau_k$, we can estimate

$$\int_0^\infty \frac{\sin(2\pi t/T)}{\pi t} e^{-t/\tau_k} dt \sim \frac{\tau_k}{T}. \tag{21}$$

After ignoring unimportant numerical prefactors, Eq. (11) yields, in agreement with Eq. (16),

$$T_{\mathrm{RMT}} \gtrsim \tau_k L. \tag{22}$$

In conclusion, we have shown that the energy scale ΔE_{RMT} at which the ETH ansatz reduces to random matrix theory has to be parametrically smaller than the inverse thermalization time, i.e., the characteristic time of the slowest mode probed by the corresponding operator. For a 1D system and a local operator A coupled to a diffusive quantity, we found ΔE_{RMT} to be bounded by $(\tau L)^{-1} \sim L^{-3}$, where L is the system size and $\tau \approx L^2/D$ is the diffusion time.

Our result (11) and (16) is an inequality, which raises the question of identifying the correct scaling of ΔE_{RMT} with the system size and understanding the significance of the associated timescale $T_{\mathrm{RMT}} = 2\pi/\Delta E_{\mathrm{RMT}}^{-1}$ from the point of view of thermalization dynamics. We conjecture that Eq. (16) reflects the correct scaling $T_{\mathrm{RMT}} \propto \tau L^d$ and propose the following interpretation. The timescale T_{RMT} which marks the onset of random matrix behavior for an observable A coincides with the end of macroscopic thermalization, i.e., applicability of the hydrodynamic description of transport. The expectation value $\delta A(t, \Psi) \sim e^{-t/\tau}$ will decay exponentially until it saturates into exponentially small fluctuations of the order of $e^{-S/2}$, where $S \propto L^d$ is entropy. This happens around time

$$T \propto \tau S, \tag{23}$$

which we conjecture to agree with T_{RMT} up to constant prefactors. This interpretation, and scaling, is consistent with the onset of RMT-defined universal behavior of the autocorrelation function at late times [38,39]. It is also consistent with the numerics shown in Fig. 2, where by the time the inequality (11) is satisfied the expectation value $\delta A(t, \Psi)$ has firmly saturated into the asymptotic fluctuation regime.

I thank Y. Bar Lev, A. Polkovnikov, and A. Shapere for reading the manuscript. I also thank the University of Kentucky Center for Computational Sciences for computing time on the Lipscomb High Performance Computing Cluster. I gratefully acknowledge support and hospitality of the Simons Center for Geometry and Physics, Stony Brook University at which part of the research for this Letter was performed. This research is supported by the National Science Foundation under Grant No. PHY-2013812.

[1] R. V. Jensen and R. Shankar, Phys. Rev. Lett. **54**, 1879 (1985).
[2] J. M. Deutsch, Phys. Rev. A **43**, 2046 (1991).
[3] M. Srednicki, Phys. Rev. E **50**, 888 (1994).
[4] M. Srednicki, J. Phys. A **29**, L75 (1996).
[5] M. Srednicki, J. Phys. A **32**, 1163 (1999).
[6] M. Rigol, V. Dunjko, and M. Olshanii, Nature (London) **452**, 854 (2008).
[7] M. Rigol and M. Srednicki, Phys. Rev. Lett. **108**, 110601 (2012).
[8] G. De Palma, A. Serafini, V. Giovannetti, and M. Cramer, Phys. Rev. Lett. **115**, 220401 (2015).
[9] L. Foini and J. Kurchan, Phys. Rev. E **99**, 042139 (2019).
[10] A. Chan, A. De Luca, and J. T. Chalker, Phys. Rev. Lett. **122**, 220601 (2019).
[11] L. Foini and J. Kurchan, Phys. Rev. Lett. **123**, 260601 (2019).
[12] M. Brenes, S. Pappalardi, M. T. Mitchison, J. Goold, and A. Silva, Phys. Rev. E **104**, 034120 (2021).
[13] W. Beugeling, R. Moessner, and M. Haque, Phys. Rev. E **89**, 042112 (2014).
[14] W. Beugeling, R. Moessner, and M. Haque, Phys. Rev. E **91**, 012144 (2015).
[15] A. Dymarsky, N. Lashkari, and H. Liu, Phys. Rev. E **97**, 012140 (2018).
[16] E. Khatami, G. Pupillo, M. Srednicki, and M. Rigol, Phys. Rev. Lett. **111**, 050403 (2013).
[17] D. J. Luitz and Y. Bar Lev, Phys. Rev. Lett. **117**, 170404 (2016).
[18] M. Serbyn, Z. Papić, and D. A. Abanin, Phys. Rev. B **96**, 104201 (2017).
[19] L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, Adv. Phys. **65**, 239 (2016).

[20] A. Altland, Y. Gefen, and G. Montambaux, Phys. Rev. Lett. **76**, 1130 (1996).

[21] M. Sonner, M. Serbyn, Z. Papić, and D. A. Abanin, Phys. Rev. B **104**, L081112 (2021).

[22] A. Dymarsky and H. Liu, Phys. Rev. E **99**, 010102(R) (2019).

[23] R. Mondaini and M. Rigol, Phys. Rev. E **96**, 012157 (2017).

[24] J. Richter, A. Dymarsky, R. Steinigeweg, and J. Gemmer, Phys. Rev. E **102**, 042127 (2020).

[25] F. Anza, C. Gogolin, and M. Huber, Phys. Rev. Lett. **120**, 150603 (2018).

[26] J. S. Cotler, G. Gur-Ari, M. Hanada, J. Polchinski, P. Saad, S. H. Shenker, D. Stanford, A. Streicher, and M. Tezuka, J. High Energy Phys. 05 (2017) 118.

[27] J. Cotler, N. Hunter-Jones, J. Liu, and B. Yoshida, J. High Energy Phys. 11 (2017) 048.

[28] L. F. Santos and E. Torres-Herrera, Nonequilibrium many-body quantum dynamics: From full random matrices to real systems, in *Thermodynamics in the Quantum Regime*, edited by F. Binder, L. Correa, C. Gogolin, J. Anders, and G. Adesso, Fundamental Theories of Physics Vol. 195 (Springer, Cham, 2018), 10.1007/978-3-319-99046-0_19.

[29] S. Moudgalya, T. Devakul, C. W. von Keyserlingk, and S. L. Sondhi, Phys. Rev. B **99**, 094312 (2019).

[30] M. Schiulaz, E. J. Torres-Herrera, and L. F. Santos, Phys. Rev. B **99**, 174313 (2019).

[31] A. Belin, J. de Boer, and D. Liska, arXiv:2110.14649.

[32] A. Belin, J. de Boer, P. Nayak, and J. Sonner, arXiv:2111.06373.

[33] C.-F. Chen and F. G. S. L. Brandão, arXiv:2112.07646.

[34] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.128.190601 for details on the numerical example and rigorous treatment of (in) equality (9).

[35] L. P. García-Pintos, N. Linden, A. S. L. Malabarba, A. J. Short, and A. Winter, Phys. Rev. X **7**, 031027 (2017).

[36] S. A. Molchanov, L. A. Pastur, and A. Khorunzhii, Theor. Math. Phys. **90**, 108 (1992).

[37] J. Wang, M. H. Lamann, J. Richter, R. Steinigeweg, A. Dymarsky, and J. Gemmer, Phys. Rev. Lett. **128**, 180601 (2022).

[38] L. V. Delacretaz, SciPost Phys. **9**, 34 (2020).

[39] T. L. M. Lezama, E. J. Torres-Herrera, F. Pérez-Bernal, Y. Bar Lev, and L. F. Santos, Phys. Rev. B **104**, 085117 (2021).