### Canonical Universality

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Isolated quantum system in a pure state may be perceived as thermal if only substantially small fraction of all degrees of freedom is probed. We propose that in a chaotic quantum many-body system all states with sufficiently small energy fluctuations are approximately thermal. We refer to this hypothesis as Canonical Universality (CU). The CU hypothesis complements the Eigenstate Thermalization Hypothesis (ETH) which proposes that for chaotic systems individual energy eigenstates are thermal. Integrable and MBL systems do not satisfy CU. We provide theoretical and numerical evidence supporting the CU hypothesis.

Consider an isolated quantum system in a pure state  $|\psi\rangle$ . We assume  $|\psi\rangle$  belongs to a sufficiently narrow energy band

$$|\psi\rangle = \sum c_n |E_n\rangle, \quad E_n \in [E - \Delta E, E + \Delta E], \quad (1)$$

where  $|E_n\rangle$  are eigenstates of energies  $E_n$ . We probe the system with an operator A, which explores only small fraction of all degrees of freedom. For example A could be acting on a substantially small subsystem of the full system. In this case Canonical Typicality [1, 2] ensures that there is a high probability that the expectation value  $\langle \psi | A | \psi \rangle$  would be approximately thermal (microcanonical)

$$\langle \psi | A | \psi \rangle \simeq \mathcal{N}^{-1} \sum A_{nn} \equiv A^{\text{micro}} ,$$
 (2)

for a typical i.e. random state (1). Corrections to (2) are suppressed by  $\mathcal{N}^{-1/2}$ , where the number of energy levels

inside the energy band  $\mathcal{N} = \int\limits_{E-\Delta E}^{E+\Delta E} \Omega \, dE$  is assumed to

be exponentially large and  $\Omega(E)$  is the density of states. Although (2) is true for most states, there might be states inside the band that are not thermal in the sense of (2), as is normally the case for energy eigenstates of integrable models.

In this paper we propose that for quantum chaotic systems all states of the form (1) with a sufficiently small  $\Delta E$  are thermal. To investigate possible deviation of  $\psi$  from thermal equilibrium (as measured by the operator A), we introduce functions  $A^{\max}$  and  $A^{\min}$  as the maximal (minimal) possible values of  $\langle \psi | A | \psi \rangle$  for all normalized states  $\psi$  of the form (1),

$$A^{\max}(E, \Delta E) = \max_{\psi} \langle \psi | A | \psi \rangle , \qquad (3)$$

$$A^{\min}(E, \Delta E) = \min_{\psi} \langle \psi | A | \psi \rangle . \tag{4}$$

Assuming discrete spectrum,  $A^{\max/\min}$  is simply maximal (minimal) eigenvalue of a hermitian  $\mathcal{N} \times \mathcal{N}$  matrix  $A_{nm}$  with n, m satisfying  $E - \Delta E \leq E_n, E_m \leq E + \Delta E$ . As such it is a monotonic function of  $\Delta E$  for fixed E. The functions  $A^{\max/\min} - A^{\min}$  specify maximal/minimal possible deviation from thermal behavior, as measured

by the operator A, for all states (1). It is then convenient to introduce function  $\Delta E(E,x)^1$  defined through

$$A^{\max}(E, \Delta E(x)) - A^{\min cro}(E) = x$$
, for  $x > 0$ , (5)  
 $A^{\min}(E, \Delta E(x)) - A^{\min cro}(E) = x$ , for  $x < 0$ . (6)

Function  $\Delta E(x)$  specifies minimal width of an energy band that includes at least one non-thermal state that exceeds some "tolerance level" x. Note that instead of  $A^{\text{micro}}$  we could also use other definition of thermal expectation value, say the canonical one. Normally we will consider x to be much larger than the ambiguity associated with different ways to define a thermal expectation value. It is convenient to normalize A rending it dimensionless. In case of finite-dimensional local Hilbert space we require ||A||=1, which limits  $|x|\leq 1$ .

Operator A could be a macro-observable associated with some extensive quantity. Qualitatively, in this case  $\Delta E(x)$  specifies minimal amount of energy fluctuations necessary to deviate from the macroscopic thermal equilibrium (MATE), as defined in [7, 8]. In case operators A are confided to a particular small subsystem, one can speak of energy fluctuations necessary to deviate from the microscopic thermal equilibrium (MITE). In the later case  $\Delta E(x)$  can be defined without referencing to a particular A. Rather, for a system in a state  $\psi$  we define reduced density matrix of the subsystem  $\rho^{\psi}$ , and introduce x via the trace distance or other approprite norm,

$$x = \max_{\psi} ||\rho^{\psi} - \rho^{\text{micro}}|| . \tag{7}$$

The maximum here is over all states (1) belonging to the band of width  $\Delta E = \Delta E(x)$ , and  $\rho^{\text{micro}}(E)$  is the reduced density matrix of the microcanonical ensemble.

We propose that in a chaotic system, for a general operator,  $\Delta E(x)$  can be described by a smooth function  $\gamma(E, x)$ , up to exponentially small corrections

$$\Delta E(E, x) = \gamma(E, x) + O\left(\Omega^{-1}\right) . \tag{8}$$

<sup>&</sup>lt;sup>1</sup> We will often suppress one of the arguments of  $\Delta E(E,x)$ , writing it simply as  $\Delta E(x)$ , whenever the implied value of E is not ambiguous.

In particular, for small x,  $\gamma(x) = \gamma_0 x^2 + \cdots$ , where for local opeartors  $g_0$  is finite and positive in the thermodynamic limit (i.e.  $V \to \infty$  with E/V kept fixed). From the definition of  $\Delta E(x)$ ,  $\gamma(x)$  should be a monotonically non-decreasing function for x>0 (and non-increasing for x<0). Coefficient  $g_0$  may exhibit different behavior: vanish or grow with volume in the thermodynamic limit. There are also operators for which g(x) grows with a smaller power as  $x\to 0$ . We will discuss such cases below. For all operators,  $\gamma(x)$  is zero only at x=0.

That  $\gamma(x)$  vanishes only at x=0 means to deviate from thermal equilibrium by a small amount x, one has to consider states built from energy eigenstates spanning a sufficiently wide interval  $\Delta E = \gamma(x) > 0$ . In particular, for the value of x below the accuracy of a measurement, all states in an energy band  $\Delta E < \gamma(x)$  are thermal. We will refer to (8) and properties of  $\gamma(x)$  as Canonical Universality (CU). While Canonical Typicality establishes that typical states from a narrow energy band are approximately thermal with an exponential precision, Canonical Universality postulates that all states from a sufficiently narrow band (1) are approximately thermal with the precision controlled by the band size  $\Delta E$ .<sup>2</sup> Clearly (8) is *not* satisfied in integrable or MBL systems, where expectation values in neighboring energy levels could differ by a finite amount, i.e.  $\Delta E(x)$  can develop characteristic plateaus  $\Delta E \sim \Omega^{-1}$  for a finite range of x (as we will later see in Fig. 1 and Fig. 4).

Smooth behavior of  $\gamma(x)$  requires that for  $\Delta E \sim \Omega^{-1}$ , x should be exponentially small. In other words, if we consider nearby states  $E_m$ , and  $E_n$ , matrix elements  $A_{mm}$  and  $A_{nn}$  must be exponentially close and  $A_{mn}$  must be exponentially small. This is reminiscent of the Eigenstate Thermalization Hypothesis (ETH)[3, 4], which proposes that matrix elements  $A_{nm}$  in energy eigenstates have a form [5]

$$A_{nm} = A^{\text{eth}}(E)\delta_{nm} + \Omega^{-1/2}(E)f(E,\omega)r_{nm} ,$$
 (9)  
 $E = (E_n + E_m)/2 , \quad \omega = (E_n - E_m) .$ 

Here  $A^{\text{eth}}$  and f are smooth function of their arguments, and "fluctuations"  $r_{nm}$  by definition have unit variance. CU (8) indirectly constrains (9) when there is an exponentially large number of states between n and m. It provides new explicit constrains once (9) is supplemented with an additional assumption about the nature of  $r_{nm}$ .

If we assume  $r_{mn}$  are independently distributed, compatibility of (8) and (9) provides a consistency condition on  $f(E,\omega)$ . It is convenient to replace  $A^{\text{micro}}$  in (5) and

(6) by  $A^{\text{eth}}(E)$ , and similarly  $\rho^{\text{micro}}$  of (7) by the universal density matrix of the subsystem ETH introduced in [9]. From the results for a band random matrix [14] one finds that  $\gamma(x)$  can be expressed in terms of f. In particular, finite and positive  $\gamma_0$  in the thermodynamic limit requires  $f(\omega)$  for fixed  $\omega$  to be volume-independent as  $V \to \infty$ . We will leave the details to supplementary material. Here to illustrate the main idea, let us consider a special case, taking  $r_{mn}$  to be a Gaussian Random Matrix compatible with the global symmetries of the problem.<sup>3</sup> Consider  $\Delta E$  to be sufficiently small so that the variance  $\sigma^2 = |f^2(E,\omega)|$  of the off-diagonal elements  $f(E,\omega)r_{nm}$ can be considered constant for  $|\omega| \leq 2\Delta E$  and the total number of energy levels inside the band (1) can be approximated as  $\mathcal{N} \approx 2\Omega \Delta E$ . In this case x of (5)–(6) are readily given by the largest (smallest) eigenvalue of the Gaussian Random Matrix  $R_{nm} = \Omega^{-1/2} f r_{nm}$  of size  $\mathcal{N}$ ,

$$x = 2\sqrt{\mathcal{N}}\Omega^{-1/2}\sigma \Rightarrow \Delta E(x) = \frac{x^2}{8\sigma^2}$$
 (10)

Clearly, the coefficient  $\gamma_0=1/(8\sigma^2)$  is positive and constant in the thermodynamic limit whenever  $\sigma^2=|f^2(E,\omega)|$  is. Relaxing that  $\sigma=f$  or  $\Omega$  are constant within the energy band will result in higher power corrections in x.<sup>4</sup>

That for generic operators f for a fixed  $\omega$  is volume independent in the thermodynamic limit can be confirmed by examining the following relation

$$\int_0^{\tau} dt \operatorname{Re}\langle A(t)A(0)\rangle_c = 2 \int_0^{\infty} dx \frac{\sin(x)}{x} \left| f\left(E, \frac{x}{\tau}\right) \right|^2 (11)$$

where  $\langle A(t)A(0)\rangle_c$  is the connected two-point function in an energy eigenstate E [10]. For A associated with non-conserved quantities one expects  $\langle A(t)A(0)\rangle_c$  to approach zero sufficiently fast, rending integral (11) finite and V-independent in the limit  $\tau \to \infty$ . This in turn implies  $|f^2|$  on the right hand side would remain finite in the thermodynamic limit.

For operators associated with conserved quantities the corresponding two-point functions can exhibit long time tail. This can make the left hand side of (11) diverge as  $\tau \to \infty$  and thus f can now develop volume dependence in the thermodynamic limit. For example, Ref. [11] suggests  $f(E,\omega \to 0)$  grow as  $L^{1/2}$  for operators with diffusive transports, where L is the typical linear size of the system.<sup>5</sup> For such operators, we may expect

<sup>&</sup>lt;sup>2</sup> Both, the typicality arguments of [1, 2] and universality, proposed in this paper, compare  $\langle \psi | A | \psi \rangle$  with the expectation of A in the microcanonical ensemble. The relation between the latter and the expectation in the canonical ensemble is a secondary issue. Hence, more accurately we should call our conjecture "microcanonical universality". Nevertheless following the terminology established in [1], we use the language of canonical universality.

<sup>&</sup>lt;sup>3</sup> This choice is suggested by both, theoretical expectations that matrix elements in a narrow shell are well represented by a Gaussian Ensemble [11], as well as numerical studies confirming Gaussian form of the distribution of  $r_{nm}$  for various non-integrable models [9, 12, 13].

<sup>&</sup>lt;sup>4</sup> For example, assuming constant f and non-zero  $T^{-1} = \partial \log \Omega / \partial E$  one can calculate next order correction to be  $\Delta E(x) = \frac{x^2}{8\sigma^2} - \frac{x^6}{3072\sigma^6T^2} + \dots$ , with higher order terms being non-universal.

<sup>&</sup>lt;sup>5</sup> It is shown in [16] that the scaling becomes anomalous  $f(E, \omega \to 0) \sim L^{(1-\alpha)/2\alpha}$  for some  $\alpha > 1/2$  in case of spatial disorder.

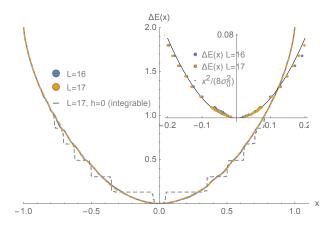


FIG. 1. Numerical plot of  $\Delta E(E=0,x)$  for operator (13) and L=16,17 in the non-integrable case h=0.1 superimposed with the integrable case L=17, h=0 (dashed line). While  $\Delta E(x)$  in the non-integrable case is smooth for all x, in the integrable case it exhibits a characteristic plateau behavior. In the limit  $L\to\infty$ , the plateau  $\Delta E\approx 0$  will stretch to at least  $|x|\simeq 0.06$ . Inset: zoomed region of small x. Numerical values for  $\Delta E(x)$  and L=16,17 and h=0.1 superimposed with the theoretical fit  $\Delta E(x)=x^2/(8\sigma_0^2)$  (black line).

 $\gamma_0 \sim L^{-1}$  in the thermodynamic limit. Physically, this can be explained as follows. Operators associated with conserved quantities exhibit stronger fluctuations as conserved quantities cannot be destroyed locally. Thus for a given deviation x from thermal equilibrium, such quantities require less energy spread compared with the generic operators. For macroscopic extensive operators below we will see numerically that  $f \propto L^{-1/2}$  (in one dimension), suggesting  $\gamma_0 \propto V$ .

Finally we note that operators of the type A=i[H,B] for some B, to which we will refer as descendant operators, exhibit different behavior from  $g(E,x)\sim x^2$ . As we discuss in supplementary materials the descendant operators must satisfy the inequality  $\Delta E(x) \geq |x|/(2|B|)$ . Thus for such operators  $\Delta E(x)$  at  $x\to 0$  increases much faster than the generic  $x^2$  behavior. This is physically sensible as such operators have zero fluctuations in an energy eigenstate and to deviate from thermal equilibrium one would need a larger amount of energy fluctuations. The examples of  $\Delta E(x)$  for the descendant operators in integrable and non-integrable cases can be found in the supplementary materials.

We illustrate different behavior  $\Delta E(x)$  with help of a nonintegrable spin-chain model with the Hamiltonian

$$H = -\sum_{i=1}^{L-1} \sigma_z^i \otimes \sigma_z^{i+1} + g \sum_{i=1}^{L} \sigma_x^i + h \sum_{i=1}^{L} \sigma_z^i , \qquad (12)$$

and  $g=1.05,\ h=0.1$ . For comparison we also present the results for an integrable model with  $g=1.05,\ h=0$ . For a given energy band, the value of  $x(E,\Delta E)$  can not be smaller than the variations of the thermal expectation value  $A^{\rm micro}(E')$  for E' inside the interval  $|E-E'| \leq \Delta E$ . In the thermodynamic limit these variations will be

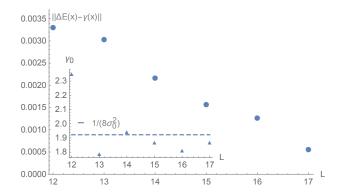


FIG. 2. Plot of  $||\Delta E(x) - \gamma(x)||$  defined in the text for operator (13), and different L = 12 - 17. Inset: plot of  $\gamma_0$  for the best fourth-order polynomial fit (for the region  $\Delta E \leq 0.2$ ) superimposed with the constant value  $1/(8\sigma_0)^2$  (dashed horizontal line).

suppressed as 1/V, which provides an upper bound on the convergence rate of  $\Delta E(E,x)$ . To minimize effects associated with finite L, we present numerical results for the local operator

$$A = \frac{g\sigma_z^1 - h\sigma_x^1}{\sqrt{g^2 + h^2}} , \quad h = 0.1 , \qquad (13)$$

which has very small variance of  $A^{\text{micro}}(E)$  in a wide range around E=0. We choose center of the band to be at E=0 at it corresponds to maximal density of states and infinite temperature (see supplementary material). The plot shown in Fig. 1, supports the conclusion that  $\Delta E(x)$  in the non-integrable case quickly becomes a smooth function, which, for small x, is well approximated by (10) with some L-independent  $\sigma=\sigma_0$ . The plot for the same operator (13) in the integrable case h=0, also shown in Fig. 1, clearly indicates  $\Delta E(x)$  remains non-smooth and exhibits a characteristic plateau at small  $\Delta E$ .

To access convergence of  $\Delta E(x)$  to a smooth  $\gamma(x)$ , we introduce the "deviation norm"  $||\Delta E(x) - \gamma(x)||$ , defined as the variance of the difference  $\Delta E_i - \gamma(x_i)$  for  $x_i = x(\Delta E_i)$ . The intervals  $\Delta E_i$  represent incremental increase of the number of levels inside the interval,  $\mathcal{N}(\Delta E_{i+1}) = \mathcal{N}(\Delta E_i) + 1$ , and  $\gamma(x)$  is a best degree four polynomial fit of  $\Delta E(x)$ . The plot in Fig. 2 shows a rapid decrease of the deviation norm with the system size, supporting (8). Numerical values of  $\gamma_0$  for different L, shown in the inset of Fig. 2, are consistent with the proposal that  $\gamma_0$  approaches a constant in the thermodynamic limit.

As we discussed earlier, if  $r_{nm}$  are random and independent,  $\gamma(x)$  becomes a function of  $f(E,\omega)$ . In particular if f is constant at small  $\omega$ ,  $\gamma_0 = 1/(8|f|^2)$ . We now test this relation numerically. For this purpose it is convenient to introduce running average variance

$$\bar{\Sigma}^2(E, \Delta E) = \frac{1}{\mathcal{N}(\mathcal{N} - 1)} \sum_{n \neq m} |A_{nm}|^2 , \qquad (14)$$

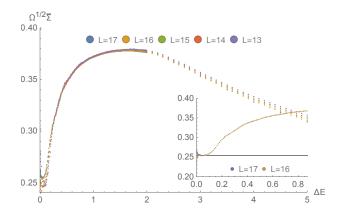


FIG. 3. Plot of  $\Omega^{1/2}(0)\bar{\Sigma}(0,\Delta E)$  for (13) and different L=13-17. Inset: plots for L=16,17 at small  $\Delta E$  superimposed with the constant value  $\sigma_0=0.255$  (horizontal line).

where the sum is over all states inside the band  $[E - \Delta E, E + \Delta E]$ . In the thermodynamic limit, when (9) applies and for sufficiently narrow  $\Delta E \gg \Omega^{-1}$ , such that  $\Omega(E)$  is approximated constant within the energy band, we have

$$\bar{\Sigma}^{2}(E,\Delta E) = \Omega^{-1}(E) \int_{-1}^{1} dt (1-|t|) \left| f(E, 2\Delta E t) \right|^{2} . (15)$$

The plot of  $\Omega^{1/2}\bar{\Sigma}(\Delta E)$  for operator (13), E=0, and different L, depicted in Fig. 3, shows that for  $\omega$  of order one  $f(0,\omega)$  quickly approaches a universal L-independent form. The same conclusion is corroborated by the analysis of two-point function  $\langle A(t)A(0)\rangle_c$  (see supplementary materials).

The inset of Fig. 3 suggests that  $\Omega(0)\bar{\Sigma}(0,\Delta E)$  at  $\Delta E \to 0$ , and hence  $f(0,\omega \to 0)$ , approach a constant  $f = \sigma_0 \approx 0.255$ . This numerical value together with (10) provide a good approximation for actual  $\Delta E(x)$ , as shown in the inset of Fig. 1. Besides,  $1/(8\sigma_0^2)$  and the value of  $\gamma_0$  we read from the best polynomial fit of  $\Delta E(x)$  are also reasonably consistent, see the inset of Fig. 2. This supports the assumption that  $r_{mn}$  are independently distributed. It is also interesting to note that  $\sigma_0^2$  is not twice smaller than the variance of the diagonal elements of  $\Omega^{-1/2}\tilde{A}_{nm}$ , as would be the case if  $\tilde{A}_{nm} = A_{nm} - A^{\text{eth}}(E)\delta_{nm}$  were a Gaussian Orthogonal Ensemble (more details are provided in the supplementary materials).

Next, we discuss CU in the context of a subsystem, when the deviation from thermal equilibrium x is defined through (7). In practice it is more convenient to define x in terms of the Frobenius norm (for a one-spin subsystem considered below these definitions coincide),

$$x^2 = \text{Tr}(\rho^{\psi} - \rho^{\text{micro}})^2 / 2 = (e^{-s_2} - e^{-s_0}) / 2$$
. (16)

Here  $\rho^{\psi}$  is the reduced density matrix of the subsystem, and  $\rho^{\text{micro}}$  is the thermal density matrix, which in case of infinite temperature is given by  $\mathbb{I}/d$  (d stand for the dimension of the Hilbert space of the subsystem). We

have also introduced  $s_2$  as the second Renyi entropy associated with the state  $\rho^{\psi}$ , while  $s_0 \equiv \log(d)$ . The definition (16) emphasizes the role of entanglement entropy as a measure of proximity of the reduced state to the thermal one. Thermal behavior is associated with the maximal volume-law entanglement  $s_2 = s_0$  and x = 0. This is in contrast to "non-thermal" energy eigenstates of integrable and MBL systems, which exhibit sub-volume entanglement.

With help of the results of [15], the problem of calculating  $\Delta E(x)$  defined through (16) can be reformulated as a maximization problem on a unit sphere  $\mathbb{S}^{d(d-1)}$ ,

$$x(\Delta E) = \max_{|\vec{c}|=1} \lambda_{\max}(\vec{c} \cdot \vec{\sigma}) / \sqrt{2d} \ . \tag{17}$$

Here  $\lambda_{\text{max}}$  denotes largest eigenvalue of a Hermitian matrix and  $\sigma^k$ , for  $k = 1 \dots d(d-1)$ , is the restriction of the full set of operators acting on the subsystem onto the energy band  $[E - \Delta E, E + \Delta E]$ .

For the subsystem consisting of one leftmost spin, d=2, and maximization in (17) can be readily performed. Numerical results for nonintegrable and integrable cases are shown in Fig. 4. In the non-integrable case  $\Delta E(x)$  exhibits a smooth behavior and is characterized by  $\propto x^2$  behavior at small x. For the integrable case  $\Delta E(x)$  is not smooth and exhibits a characteristic plateau near  $\Delta E=0$ .

Finally, we consider two extensive operators characterizing full magnetization,  $A_{x/z} = \frac{1}{L} \sum_{i=1}^{L} \sigma_{x/z}^{i}$ . The corresponding plots of  $\Delta E(x)$  and  $\bar{\Sigma}$  are shown in supplementary materials. In the non-integrable case  $\Delta E(x)$  is smooth with the characteristic  $\propto x^2$  behavior at the origin. On the contrary, in the integrable case  $\Delta E(x)$  demonstrates a characteristic plateau near  $\Delta E \approx 0$ . The plots for  $L^{1/2}\Omega^{1/2}\bar{\Sigma}$  demonstrate L-independent behavior, which indicates  $f(0,\omega)$  for fixed  $\omega$  scales as  $L^{-1/2}$ . This scaling tentatively suggests  $\Delta E(x)$  will scale with

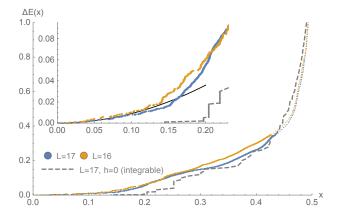


FIG. 4. Numerical plot of  $\Delta E(E=0,x)$  (17) for the subsystem consisting of one leftmost spin i=1. Data points for L=16,17 for non-integrable h=0.1 case superimposed with the integrable model L=17,h=0 results (dashed line). Inset: zoomed region of small x superimposed with  $x^2$  fit.

the volume such that  $\Delta E(x)/V$  will remain finite in the thermodynamic limit.

Let us summarize our findings. We argued that for quantum chaotic system, all states from a sufficiently narrow energy band must be approximately thermal in terms of microscopic and macroscopic equilibrium. This behavior, which we refer to as Canonical Universality, can be quantified in terms of function  $\Delta E(x)$  that specifies

maximal deviation from thermal equilibrium for states from a narrow energy band. We argued that in the chaotic case for a general operator  $\Delta E(x) = \gamma(x)$  becomes smooth and exhibits  $\propto x^2$  behavior for small x. We provided analytical and numerical evidence that for local operators not associated with any conserved quantities  $\Delta E(x)$  remain finite in the thermodynamic limit, while for the extensive operators the same applies to  $\Delta E(x)/V$ .

- S. Goldstein, J. Lebowitz, R. Tumulka, and N. Zanghi, "Canonical typicality," Physical review letters 96, no. 5 (2006): 050403, [arXiv:cond-mat/0511091].
- [2] S. Popescu, A. Short, A. Winter, "Entanglement and the foundations of statistical mechanics," Nature Physics, (2006): 2(11), 754-758, [arXiv:quant-ph/0511225].
- [3] J. Deutsch, "Quantum statistical mechanics in a closed system," Physical Review A 43, no. 4 (1991): 2046.
- [4] Srednicki, "Chaos and quantum thermalization," Physical Review E 50, no. 2 (1994): 888.
- [5] M. Srednicki, "The approach to thermal equilibrium in quantized chaotic systems," Journal of Physics A: Mathematical and General 32.7 (1999): 1163.
- [6] M. Rigol, V. Dunjko, and M. Olshanii, "Thermalization and its mechanism for generic isolated quantum systems," Nature, (2008): 452(7189), 854-858, [arXiv:0708.1324].
- [7] S. Goldstein, D. Huse, J. Lebowitz, R. Tumulka, "Thermal equilibrium of a macroscopic quantum system in a pure state," Physical Review Letters. 2015 Sep. 4;115(10):100402, [arXiv:1506.07494].
- [8] S. Goldstein, D. Huse, J. Lebowitz, R. Tumulka, "Macroscopic and Microscopic Thermal Equilibrium," [arXiv:1610.02312]
- [9] A. Dymarsky, N. Lashkari, H. Liu, "Subsystem ETH", [arXiv:1611.08764].
- [10] E. Khatami, G. Pupillo, M. Srednicki, M. Rigol, "Fluctuation-Dissipation Theorem in an Isolated System of Quantum Dipolar Bosons after a Quench," Phys. Rev. Lett. 111, 050403 (2013), [arXiv:1304.7279].
- [11] L. D'Alessio, Y. Kafri, A. Polkovnikov, M. Rigol, "From Quantum Chaos and Eigenstate Thermalization to Statistical Mechanics and Thermodynamics," Adv. Phys. 65, 239 (2016), [arXiv:1509.06411].
- [12] W. Beugeling, R. Moessner, and M. Haque, "Finite-size scaling of eigenstate thermalization," Phys. Rev. E 89, 042112 (2014), [arXiv:1308.2862].
- [13] W. Beugeling, R. Moessner, M. Haque, "Off-diagonal matrix elements of local operators in many-body quantum systems," Phys. Rev. E 91, 012144 (2015), [arXiv:1407.2043].
- [14] S. Molchanov, L. Pastur, and A. Khorunzhii, "Limiting eigenvalue distribution for band random matrices," Theoretical and Mathematical Physics 90, no. 2 (1992): 108-118.
- [15] A. Dymarsky, "Convexity of a Small Ball Under Quadratic Map," Linear Algebra and Its Applications, Volume 488, (2016), p. 109123, [arXiv:1410.1553].
- [16] D. Luitz, Y. Lev, "Anomalous thermalization in ergodic systems," Phys. Rev. Lett. 117, 170404 (2016), [arXiv:1607.01012].

### Supplementary Materials: Canonical Universality

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#### I. BAND RANDOM MATRICES

Let us consider an energy band of width  $2\Delta E$  centered around E. We will keep  $\Delta E$  and E/V fixed, while volume grows  $V \to \infty$ . Assuming the system admits thermodynamic limit, both  $A^{\text{eth}}(E)$  and  $f(E,\omega)$  introduced in (9) are expected to smoothly depend on E only through temperature T = T(E/V). Hence one can approximate  $(E_n + E_m)/2$  by the median energy of the band E. With an additional assumption that  $\Delta E$  is narrow enough such that the density of states  $\Omega$  within the band is approximately constant, (9) can be rewritten as follows,

$$A_{nm} - A^{\text{eth}}(E)\delta_{nm} = \frac{\sqrt{2\Delta E}}{\mathcal{N}^{1/2}}v\left(\frac{n-m}{\mathcal{N}}\right)r_{nm} , (18)$$
$$v^{2}(t) = |f^{2}(E, 2t\Delta E)| , |t| \leq 1 , \mathcal{N} = 2\Omega\Delta E .$$

Assuming independent nature (but not necessarily Gaussian form) of random variables  $r_{nm}$ , equation (18) defines a band random matrix  $\tilde{A}_{nm} = (A_{nm} - A^{\text{eth}}(E))/\sqrt{2\Delta E}$ , which was studies by Molchanov, Pastur, and Khorunzhii in [14]. Namely, they consider a band random matrix  $\tilde{A}_{nm}$ ,  $n, m = 1, ..., \mathcal{N}$ , with all elements being independently distributed, and the variance specified by an even function  $v^2(t)$ ,

$$\langle |\tilde{A}_{nm}|^2 \rangle = \mathcal{N}^{-1} v^2 \left( \frac{n-m}{\mathcal{N}} \right) .$$
 (19)

Under some technical assumptions, the generating function

$$r(x) = \frac{1}{\mathcal{N}} \operatorname{Tr} \frac{1}{x - \tilde{A}} , \qquad (20)$$

can be expressed in terms of an auxiliary function  $r(x) = \int_{-1/2}^{1/2} r(t, x) dt$ ,

$$r(t,x) = -\sum_{i=0}^{\infty} \frac{a_i(t)}{x^{2i+1}}, \quad a_0(t) = 1,$$
 (21)

while the latter satisfies a particular integral equation. This integral equation can be rewritten as a system of recursive relations for  $a_k(t)$ ,

$$a_{k+1}(t) = \sum_{p=0}^{k} a_p(t) \int_{-1/2}^{-1/2} v^2(t-t') a_{k-p}(t') dt' . (22)$$

These equations can be solved perturbatively. Assuming  $v^2(t)$  is almost constant,  $v^2(t) = v_0^2 + \delta v^2(t)$ , we perform

a formal expansion in powers of  $\delta v^2$ ,

$$\int_{-1/2}^{1/2} a_k(t)dt = 4^k \frac{\Gamma(k+1/2)}{(k+1)!\sqrt{\pi}} \left(v_0^2 + u_1 + u_2/v_0^2 + \dots\right)^k ,$$

$$u_1 = \int_{-1/2}^{1/2} dt \int_{-1/2}^{1/2} dt' \, \delta v^2(t-t') ,$$

$$u_2 = -2 \left(\int_{-1/2}^{1/2} dt \int_{-1/2}^{1/2} dt' \, \delta v^2(t-t')\right)^2 +$$

$$2 \int_{-1/2}^{1/2} dt \int_{-1/2}^{1/2} dt' \int_{-1/2}^{1/2} dt'' \, \delta v^2(t-t') \delta v^2(t'-t'') .$$

Here  $u_1$  is linear in  $\delta v^2$ ,  $u_2$  is quadratic and so on. Expansion (21) became divergent at  $x = \pm 2(v_0^2 + u_1 + \dots)$ , which is the value of largest/smallest eigenvalue of  $\tilde{A}$ . Going back to (18), one can express  $x(\Delta E)$  as

$$\Delta E(x) = x^2 / (8\sigma_v^2) , \qquad (23)$$

where the higher order terms in x are implicitly absorbed into a single coefficient  $\sigma_v(\Delta E(x))$ ,

$$\sigma_v^2 = v_0^2 + \int_{-1}^1 \delta v^2(t) (1 - |t|) dt + \mathcal{O}(\delta v^2) \ . \tag{24}$$

It is interesting to note that up to linear in  $\delta v^2$  term, (24) coincides with the integral in (15). Hence, when  $f(E,\omega)$  is almost constant,  $\sigma_v^2$  can be approximated as  $\Omega \bar{\Sigma}^2(\Delta E)$ .

# II. CANONICAL UNIVERSALITY FOR OPERATORS A = i[H, B]

Consider an operator A of the form

$$A = i[H, B] , \qquad (25)$$

for some B and the Hamiltonian H. If H includes only local interactions and B acts on a small sub-system then A would be localized as well. Operators of the form (25), which we call "descendants", are special in the sense that they trivially satisfy ETH,

$$\langle E_n | A | E_n \rangle = 0 , \qquad (26)$$

which means  $A^{\rm eth}=0$  for any E. Furthermore for any pure state  $\psi$  of the form (1),

$$x = \langle \psi | A | \psi \rangle = -i \langle \psi | B | \psi_1 \rangle + \text{c.c} ,$$
 (27)

where  $\psi_1 = (H - E)\psi$ . Consequently, |x| is bound from above by

$$|x| \le 2|B|\Delta E , \qquad (28)$$

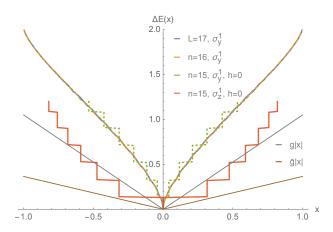


FIG. 5. Plots of  $\Delta E(E=0,x)$  for  $\sigma_y^1$  and L=16,17 in the non-integrable case (blue, yellow), and L=15 in the integrable case h=0 (green). Also, plot of  $\Delta E(E=0,x)$  for  $\sigma_z^1$  and L=15 in the integrable case h=0 (red). Superimposed with the theoretical bound g|x| (gray) and  $\tilde{g}|x|$  (brown).

where we used  $|\psi_1| \leq \Delta E$ . This leads to the bound

$$\Delta E(x) \ge \frac{|x|}{2|B|} \ . \tag{29}$$

We plot  $\Delta E(x)$  for  $A=\sigma_y^1=i[H,\sigma_z^1/(2g)]$  together with the bound g|x| in the integrable and non-integrable case in Fig. 5. It turns out the operator  $\sigma_z^1$  in the integrable case is also a descendant. The corresponding B is non-local and

$$(2|B|)^{-1} =: \tilde{g}(L) = g\sqrt{\frac{1 - g^{-2}}{1 - g^{-2L}}}$$
 (30)

Notice, that  $\tilde{g}$  is finite in the infinite volume limit  $L \to \infty$ , and hence  $\Delta E(x)$  can not be smooth at  $x \to 0$ . We plot  $\Delta E(x)$  for  $\sigma_z^1$  and the corresponding theoretical bound in Fig. 5. In fact  $\sigma_z^i$  for any i in the integrable case is a descendant, and so is the average magnetization operator  $A_z = \sum_i^L \sigma_z^i / L$ . In the latter case the norm of |B| grows with L, and therefore the bound (29) becomes obsolete in the thermodynamic limit. The plot for  $A_z$  (Fig. 12) suggests that despite integrability  $\Delta E(x)$  actually becomes a smooth function of x with the characteristic  $\propto x^2$  behavior at small x. This is reminiscent of observation that macroscopic observables are thermal in most eigenstates for both chaotic and non-chaotic systems [7, 8].

#### III. DENSITY OF STATES

The non-integrable model (12) was numerically studied in [9]. There it was observed that the density of states is well approximated by the binomial distribution

$$\Omega_n(E) = \frac{\kappa L!}{(L/2 - \kappa E)!(L/2 + \kappa E)!} , \qquad (31)$$

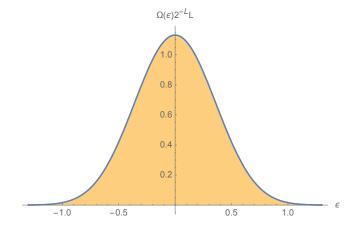


FIG. 6. Density of states of the spin chain (12) with g=1.05, h=0.1, L=17. The horizontal axis is energy per site  $\epsilon=E/L$ . Yellow bars which is the histogram of the actual density of states calculated using direct diagonalization. The blue solid line is a theoretical fit by the binomial distribution function (31) with  $\kappa\approx0.3489$ .

with  $\kappa$  given by

$$\kappa = \frac{1}{2} \left( g^2 + h^2 + 1 - 1/L \right)^{-1/2} . \tag{32}$$

The actual density of states and the theoretical fit (31) for L=17 are depicted in Fig. 6. The expression for the density of states (31) was used to determine  $\Omega^{1/2}\bar{\Sigma}$  shown in Fig. 3, Fig. 9, and Fig. 14. When L becomes large  $\Omega(0)$  can be approximated as

$$\Omega(0) = \frac{2^L L^{-1/2}}{\sqrt{2\pi} \sqrt{g^2 + h^2 + 1}} \ . \tag{33}$$

The factor  $L^{-1/2}$  contributes to the correct scaling behavior of  $f(E=0,\omega)$ .

#### IV. CHOICE OF OPERATOR A

For a given energy band, the value of  $x(E,\Delta E)$  can not be smaller than the variations of the thermal expectation values  $A^{\text{micro}}(E')$  or  $A^{\text{eth}}(E')$  for E' inside the interval  $|E-E'| \leq \Delta E$ . Since in the chaotic case  $A^{\text{eth}}(E)$  is a smooth function of E, these variations are of the order  $\Delta E dA^{\text{eth}}/dE$  and are expected to be suppressed as 1/V in the thermodynamic limit. To minimize finite-size effects affecting  $\Delta E(x)$  we would like to identify an operator A which has small value of  $dA^{\text{eth}}/dE$ . Looking at the one-spin operators acting on the leftmost spin (see Fig. 7) we observe that  $A^{\text{eth}}(E)$  for both  $\sigma_z^1$  and  $\sigma_x^1$  are approximately linear function of E with some non-zero slope, such that the combination (13) has almost vanishing expectation value for a wide range of E around E=0.

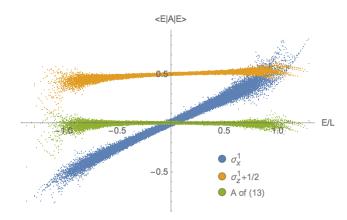


FIG. 7. Expectation values  $\langle E_n|A|E_n\rangle$  for  $A=\sigma_x^1$ ,  $A=\sigma_z^1$ , and A given by (13) in case of L=17 as a function of  $E_n/L$ .

#### V. TWO-POINT FUNCTION $\langle A(t)A(0)\rangle_c$

Function  $f(E,\omega)$  can be constrained through the behavior of the connected the two-point function [10, 11],

$$\langle E_n | A(t) A(0) | E_n \rangle_c = \sum_{m \neq n} e^{i(E_n - E_m)t} |A_{nm}|^2$$
. (34)

Assuming (9), in the continuous limit the integral of the two-point function can be rewritten as follows

$$\begin{split} & \int_0^\tau dt \, \Re \langle E_n | A(t) A(0) | E_n \rangle_c = \\ & \int_{-\infty}^\infty d\omega \frac{\sin(\omega \tau)}{\omega} \frac{\Omega(E_n + \omega/2)}{\Omega(E_n)} f(E_n + \omega/2, \omega) |^2 \; . \end{split}$$

Because of oscillatory behavior of  $\frac{\sin(\omega\tau)}{\omega}$ , only values of  $|\omega| \lesssim 1/\tau$  contribute to the integral. When the temperature associated with  $E_n$  is infinite, one can neglect  $\omega$ -dependence in  $E_n + \omega/2$  inside  $\Omega$  and f, so far  $|\omega| \ll L^{1/2}$ ,

$$\int_0^{\tau} dt \operatorname{Re}\langle A(t)A(0)\rangle_c = 2 \int_0^{\infty} d\omega \frac{\sin(\omega \tau)}{\omega} |f(E,\omega)|^2$$
 (35)

This relation is valid for  $\tau \gg L^{-1/2}$ . Here we introduced the notations  $\langle A(t)A(0)\rangle_c$  for  $\langle E|A(t)A(0)|E\rangle_c$  when energy E corresponds to infinite temperature  $d\Omega/dE=0$ . Numerically, we define  $\langle A(t)A(0)\rangle_c$  by averaging over hundred states in the middle of the spectrum,

$$\langle A(t)A(0)\rangle_c = \frac{1}{100} \sum_{n=2^L/2-49}^{2^L/2+50} \langle E_n|A(t)A(0)|E_n\rangle_c$$
 (36)

## VI. ANALYSIS OF $\bar{\Sigma}$ AND $\langle A(t)A(0)\rangle_c$ FOR DIFFERENT OPERATORS

Here we provide additional details of the analysis of the numerical results. Based on the plot for  $\bar{\Sigma}$  in the

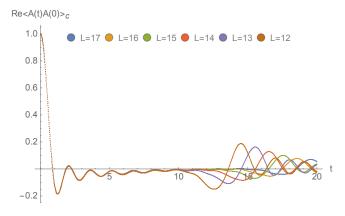


FIG. 8. Plot of  $\text{Re}\langle A(t)A(0)\rangle_c$  defined in (36) for operator (13) and different L=12-17.

main text (Fig 3) we concluded  $f(0,\omega)$  for  $\omega$  of order one should be L independent. The same conclusion can be reached from the analysis of two-point function  $\langle A(t)A(0)\rangle_c$  shown in Fig. 8. In this case temperature is formally infinite, and therefore (35) applies so far  $\tau\gg L^{-1/2}$ . Numerical plot clearly shows that the two-point function quickly converges to an L-independent form for  $0 \le t \le t^*(L)$ , where  $t^* \sim L$  is the time of the "rebound" when the finite-size effects become important. Hence for substantially large L, any fixed  $\tau$  would satisfy  $L^{-1/2} \ll \tau \ll L$ , rendering the integral (11) L-independent. This confirms L-independence of  $f(E,\omega)$ .

When  $\Delta E \to \infty$  the behavior of  $\bar{\Sigma}(\Delta E)$  can be deduced from the inequality

$$\bar{\Sigma}^2(\Delta E) \le \frac{\text{Tr}(A^2)}{\mathcal{N}(\mathcal{N} - 1)} , \qquad (37)$$

and an explicit form of  $\Omega$  (33). When  $\Delta E$  is so large that the band includes almost all states,  $\Omega^{-1/2}(0)\bar{\Sigma}(0,\Delta E)$  goes to zero as  $L^{-1/2}$ .

The limit of small  $\Delta E \to 0$  is more difficult to probe. For  $t \geq t^*(L)$  the behavior of  $\langle A(t)A(0)\rangle_c$  is not universal, hence we can not immediately use (35) to bound  $f(0,\omega)$  in the region of small  $\omega \sim L^{-1}$ . The plot of  $\Omega^{-1/2}\bar{\Sigma}(\Delta E)$  suggests f approaches a constant  $f(0,\omega \to 0) = \sigma_0 \sim 0.255$  (see the inset of Fig. 3). It is nevertheless possible that in a small region of size  $L^{-1}$  or less,  $f(E,\omega)$  grows with L.

Next, we analyze the one-spin operator  $A = \sigma_x^1$ . The corresponding plots for  $\bar{\Sigma}$  (Fig. 9) and  $\langle A(t)A(0)\rangle_c$  (Fig. 10) support the same conclusion as above:  $f(0,\omega)$  is L independent in the thermodynamic limit. The plot of  $\Delta E(x)$  for  $\sigma_x^1$  in the integrable and non-integrable case is shown in Fig. 11. In the non-integrable case function  $\Delta E(x)$  becomes smooth and is reasonably described by (10) at small x. The corresponding value of  $\sigma_0 \approx 0.58$  is determined as the limit of  $f(0,\omega)$  as  $\omega$  approaches zero, see the inset of Fig. 9. The plot for integrable case exhibits a characteristic plateau at  $\Delta E \approx 0$ . Using free fermion representation of the integrable model (12) with

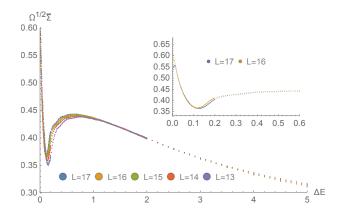


FIG. 9. Plot of  $\Omega^{1/2}(0)\bar{\Sigma}(0,\Delta E)$  for  $A=\sigma_x^1$  and different L=13-17. Inset: plots for L=16,17 and small  $\Delta E$ . The limit of  $\Omega^{1/2}(0)\bar{\Sigma}(0,\Delta E)$  as  $\Delta E$  approaches zero is approximately equal to  $f(0,\omega\to 0)=\sigma_0\approx 0.57$ .

h=0, one can show the plateau at  $\Delta E\approx 0$  in the thermodynamic limit  $L\to\infty$  must stretch to at least  $|x|\approx 0.64$ . This also implies the plateau at Fig. 1 will stretch to at least  $|x|\approx 0.06$ .

As a last step we analyze extensive operators  $A_{x/z} = \sum_i \sigma_{x/z}^i / L$ . The plots of  $\Delta E(x)$  for integrable and non-integrable cases is shown in Fig. 12. In the non-integrable case  $\Delta E(x)$  for both operators is smooth and is  $\propto x^2$  at small x. In the integrable case  $\Delta E(x)$  for  $A_x$  develops a characteristic plateau near  $\Delta E \approx 0$  and is not smooth. The plot of  $\Delta E(x)$  for  $A_z$  in the integrable case is smooth and qualitatively indistinguishable from the non-integrable case, which we assume is the consequence of  $A_z$  being a descendant operator. The plot of  $\bar{\Sigma}$  for  $A_{x/z}$  (Fig. 14) clearly shows  $L^{1/2}\Omega^{1/2}(0)\bar{\Sigma}(0,\Delta E)$  is L-independent, hence suggesting the scaling  $f(0,\omega) \sim L^{-1/2}$ .

#### VII. VARIANCE OF $A_{nm}$

It was observed in [9] that in the model in question the fluctuations of the diagonal matrix elements  $A_{nn}$  of local operators, e.g. one-spin operator (13), are well described by the Gaussian distribution. The procedure of calculating  $A^{\text{eth}}(E)$  and the variance  $\langle R_{nn}^2 \rangle$  of  $R_{nm} = \Omega^{1/2}(0)(A_{nm} - A^{\text{eth}}(E_n)\delta_{nm})$  is described in [9]. Here we show the histogram of distribution of  $R_{nn}$  inside a central band superimposed with the Gaussian fit, see Fig. 13. The value of variance  $\langle R_{nn}^2 \rangle$  for (13) and the systems consisting of L = 12 - 17 spins is shown in Fig. 15. It is approximately L independent,  $\langle R_{nn}^2 \rangle^{1/2} \approx 0.418$ . Assuming matrix elements  $R_{nm}$  inside a narrow energy band form the Orthogonal Gaussian Ensemble, variance of the off-diagonal elements, which was found in the text to be  $\langle R_{nm}^2 \rangle = \sigma_0^2 \sim 0.255^2$  (see the inset of Fig. 1), should be twice smaller than  $\langle R_{nn}^2 \rangle$ . But this does not

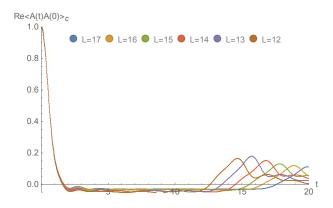


FIG. 10. Plot of  $\text{Re}\langle A(t)A(0)\rangle_c$  defined in (36) for operator  $A=\sigma_x^1$  and different L=12-17.

seem to be the case:

$$\begin{split} 2^{1/2} \langle R_{nm}^2 \rangle^{1/2} &= 2^{1/2} \sigma_0 \approx 0.361 \ , \\ \langle R_{nn}^2 \rangle^{1/2} &\approx 0.418 \ . \end{split}$$

This discrepancy is illustrated in Fig. 15.

## VIII. CALCULATION OF $\Delta E(x)$ FOR A SUBSYSTEM

For a subsystem of arbitrary size and energy E associated with infinite temperature, we define deviation from the microscopic thermal equilibrium by comparing reduced density matrix  $\rho^{\psi}$  with the thermal one  $\rho^{\text{th}} = \mathbb{I}/d$ ,

$$x^2 = \frac{1}{2} \operatorname{Tr}(\rho^{\psi} - \rho^{\text{th}})^2 = (e^{-s_2(x)} - e^{-s_0})/2$$
, (38)

$$s_2 = -\log \text{Tr} \left[ (\rho^{\psi})^2 \right] , \quad s_0 = \log d . \quad (39)$$

Here d is the dimension of the Hilbert space of the subsystem and  $s_2$  - second Renyie entropy. To calculate x as

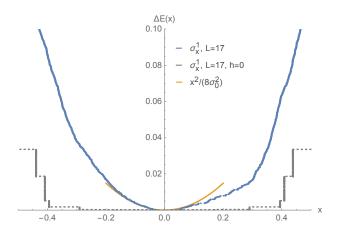


FIG. 11. Plots of  $\Delta E(0,x)$  for operators  $\sigma_x^1$  for integrable h=0 (gray dashed line) and non-integrable h=0.1 (blue dots) cases and L=17, superimposed with the theoretical fit (10) and value of  $\sigma_0 \approx 0.58$  (see the inset of Fig. 9).

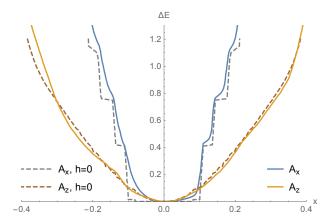


FIG. 12. Plots of  $\Delta E(0,x)$  for operators  $A_x$  and  $A_z$  for integrable h=0 (dashed lines) and non-integrable h=0.1 (solid lines) cases and L=17.

a function of state  $\psi$  we introduce a full set of traceless Hermitian operators acting on the subsystem  $\hat{\sigma}_k$ ,  $k = 1, \ldots, d(d-1)$ ,  $\operatorname{Tr} \hat{\sigma}_k = 0$ ,  $\operatorname{Tr}(\hat{\sigma}_k \hat{\sigma}_\ell) = d\delta_{k\ell}$ . In case of the subsystem consisting of one spin, d = 2 and  $\hat{\sigma}_k$  are simply Pauli matrices  $\sigma_k$ . Then  $x(\psi)$  is given by

$$2dx^{2} = \sum_{k=1}^{d(d-1)} \text{Tr}(\rho^{\psi} \hat{\sigma}_{k})^{2} . \tag{40}$$

To find  $x(\Delta E)$  we need to maximize (40) over all  $\psi$  of the form (1). Numerically it can be done by introducing  $\mathcal{N} \times \mathcal{N}$  matrices  $(\sigma_k)_{nm} = \langle E_n | \hat{\sigma}_k | E_m \rangle$ , and using Lemma 2 from [15] to reduce the original problem to an optimization problem on a sphere,  $\vec{c} \in \mathbb{S}^{d(d-1)}$ ,

$$x(\Delta E) = \frac{\max_{|\vec{c}|=1} \lambda_{\max}(\vec{c} \cdot \vec{\sigma})}{\sqrt{2d}} . \tag{41}$$

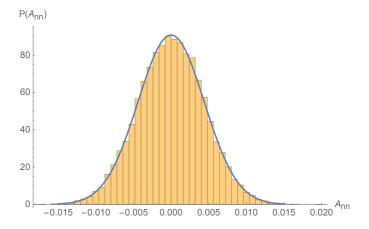


FIG. 13. Histogram of probability distribution of  $A_{nn}$  for operator (13) from the central band,  $E=0, \Delta E=0.1L$ , for the spin-chain consisting of L=17 spins. Superimposed blue line is the normal distribution with the same mean and variance.

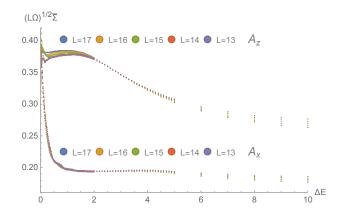


FIG. 14. Plot of  $\Omega^{1/2}(0)\bar{\Sigma}(0,\Delta E)$  for operators  $A_z$  (group of lines at the top) and  $A_x$  (group of lines at the bottom), and different L=13-17.

Here  $\lambda_{\max}(\sigma)$  is the largest eigenvalue of a Hermitian matrix  $\sigma$ . In case of the leftmost spin, vector  $\vec{c} \in \mathbb{S}^3$  can be conventionally parametrized with help of two angles

$$\vec{c} \cdot \vec{\sigma} = \cos \theta \, \sigma_x^1 + \sin \theta \cos \phi \, \sigma_z^1 + \sin \theta \sin \phi \, \sigma_y^1 \ . \tag{42}$$

Maximization over  $0 \le \theta \le \pi$  and  $0 \le \phi \le \pi$  (it is enough to cover only half-sphere because  $\lambda_{\max}(\sigma) = \lambda_{\max}(-\sigma)$ ) can be done by introducing a discretization of both intervals and then scanning through all possible values. Numerical calculations for all considered  $\Delta E$  and L shows that maximum of  $\lambda_{\max}(\vec{c}\cdot\vec{\sigma})$  is achieved at  $\phi=0$ . This is presumably related to the fact that  $\sigma_y^1$  is a descendant operator and requires more energy fluctuations to deviate from thermal equilibrium. This observation substantially simplifies calculations as it reduced the problem of finding global maximum to optimization with respect to one only parameter  $\theta$ . The latter problem can be solved in a variety of ways, e.g. with help of Newton's method using analytic expression for the gradient  $d\lambda_{\max}(\vec{c}\cdot\vec{\sigma})/d\theta$  in terms of eigenvectors of  $\vec{c}\cdot\vec{\sigma}$ .

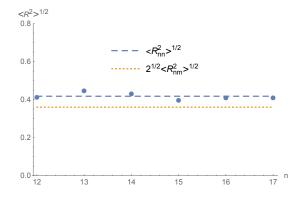


FIG. 15. Variance of matrix elements  $R_{nn}$  for operator (13) and  $E_n$  from the central band E=0,  $\Delta E=0.1L$ , plotted for different values of L=12-17. Blue dashed line: mean value  $\langle R_{nn}^2 \rangle^{1/2} \approx 0.418$ . Dotted orange line: the value of  $2^{1/2} \langle R_{nm}^2 \rangle^{1/2} = 2^{1/2} \sigma_0 \approx 0.361$ .