Dynamical Typicality Approach to Eigenstate Thermalization

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We consider the set of all initial states within a microcanonical energy shell of an isolated many-body quantum system, which exhibit an arbitrary but fixed nonequilibrium expectation value for some given observable A. On the condition that this set is not too small, it is shown by means of a dynamical typicality approach that most such initial states exhibit thermalization if and only if A satisfies the so-called weak eigenstate thermalization hypothesis (wETH). Here, thermalization means that the expectation value of A spends most of its time close to the microcanonical value after initial transients have died out. The wETH means that, within the energy shell, most eigenstates of the pertinent system Hamiltonian exhibit very similar expectation values of A.

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The eigenstate thermalization hypothesis (ETH) plays a pivotal role in numerous recent investigations of thermalization in isolated many-body quantum systems [1,2], comparable to the role of the ergodic hypothesis in the classical realm. In essence, the ETH postulates that energy eigenstates with sufficiently close energy eigenvalues exhibit very similar expectation values [3–6]. It is generally taken for granted that the ETH guarantees thermalization for any initial state with a macroscopically well-defined system energy. Whether the ETH is also necessary for thermalization is a question of considerable current interest [2,7–13]. Here, we will provide examples implying that the ETH (in its most common version) should be considered neither as sufficient nor as necessary for thermalization without any further specification of the admitted initial states.

Accordingly, we will focus on a suitable subset of initial states, namely, all pure states which exhibit the same arbitrary but fixed initial expectation value for some given observable A. In the most common case, this subset is still "reasonably large" (in a mathematically precisely defined sense) and entails quite remarkable dynamical typicality and concentration of measure properties, as detailed in Refs. [14,15]. Here, we further develop these concepts and show that a "weak" version of the ETH [16–20] is both necessary and sufficient in order that the vast majority of those initial states exhibit thermalization with respect to the observable A at hand. Whether or not a given system thermalizes and whether or not it satisfies the ETH are very important issues in themselves, but they are not at the focus of our present work. Rather, our main focus is on how the two issues are connected.

Based on related preliminary conjectures [21,22], the ETH was originally proposed in the context of chaotic systems in the semiclassical limit [4,5]; see also [23–26]. In fact, for so-called macroscopic observables, the ETH is already buried in von Neumann's work [27,28], as pointed out in Refs. [8,29–31]. More recent analytical investigations of the ETH often focus on (sums of) local observables, subsystems in contact with a heat bath, spatially discrete lattice models, or Hamiltonians with bound spectra [7,9,10,12,16]. In view of the quite extensive numerical explorations [1,2] and of Deutsch's results based on random matrix theory [3,32], this Letter pursues the standpoint that the ETH is an interesting and relevant concept beyond any such particular class of systems and observables.

As usual [1,2], the isolated many-body system is described by a Hamiltonian H with discrete eigenvalues E_n and eigenvectors $|n\rangle$. Focusing on an arbitrary but fixed microcanonical energy interval $[E-\epsilon, E]$, the number of energies E_n in this interval is denoted by N, and we choose the indices so that $n \in \{1,\ldots,N\}$ for all those E_n's. The width ϵ is assumed to be small on the macroscopic scale (well-defined system energy) but large on the microscopic scale. For many-body systems with $f \gg 1$ degrees of freedom, N is then exponentially large in f [28]. The energy eigenstates $\{|n\rangle\}_{n=1}^{N}$ span a Hilbert space $\mathcal{H}$, called the microcanonical energy shell.

Considering any given $|\psi\rangle \in \mathcal{H}$ as an initial state $|\psi(0)\rangle$, it evolves in time according to $|\psi(t)\rangle = U_t|\psi\rangle$ with $U_t := e^{-iHt/\hbar}$, yielding for an arbitrary observable A the expectation value

$$\langle\psi(t)|A|\psi(t)\rangle = \langle\psi|A_t|\psi\rangle, \tag{1}$$

$$A_t := U_t^\dagger A U_t = \sum_{m,n=1}^{N} A_{mn} e^{i(E_m-E_n)t/\hbar}|m\rangle\langle n|, \tag{2}$$

where $A_{mn} := \langle m|A|n\rangle$. In cases where the Hamiltonian H exhibits degeneracies, its eigenvectors $|n\rangle$ are chosen so

that the matrix A_{mn} is diagonal within every eigenspace. Denoting averages over all times $t \geq 0$ by an overbar, it follows that

$$\overline{A_t} = \sum_{n=1}^{N} A_{nn} |n\rangle\langle n|, \tag{3}$$

and for the time-averaged expectation value in (1) that

$$A_\psi := \overline{\langle\psi(t)|A|\psi(t)\rangle} = \langle\psi|\overline{A_t}|\psi\rangle = \sum_{n=1}^{N} |\langle n|\psi\rangle|^2 A_{nn}. \tag{4}$$

The most common or "strong" version of ETH (sETH) states [1,2] that the diagonal matrix elements A_{nn} assume very similar values for all $n \in \{1, \ldots, N\}$. Consequently, the long time average in (4) is very well approximated by the microcanonical expectation value $A_{\mathrm{mc}} := \mathrm{Tr}\{\rho_{\mathrm{mc}} A\}$, where $\rho_{\mathrm{mc}} := I_{\mathcal{H}}/N$ and $I_{\mathcal{H}} := \sum_{n=1}^{N} |n\rangle\langle n|$ (identity on $\mathcal{H}$). Since this is precisely the prediction of textbook statistical mechanics for our system at thermal equilibrium, and since this property applies to any initial condition $|\psi\rangle \in \mathcal{H}$, it is tempting to conclude that the sETH implies thermalization. However, one can readily tailor initial conditions and observables, which fulfill the sETH and $A_\psi \simeq A_{\mathrm{mc}}$, while the expectation values in (1) maintain non-negligible oscillations *ad infinitum*; i.e., they do not exhibit thermalization in any meaningful sense. For example, $|\psi\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$, $A_{12} = A_{21} = 1$, and $A_{mn} = 0$ for all other m, n yields $\langle\psi(t)|A|\psi(t)\rangle = \cos(\omega t)$ with $\omega := (E_2 - E_1)/\hbar$. One may object that this example is experimentally unrealistic [33] and incompatible with the generalized ETH postulated in Ref. [5], yet there seems to be no argument which *rigorously* disqualifies *all* counterexamples of this kind. Accordingly, the sETH should not be considered as sufficient for thermalization without any further conditions regarding the observables or the initial conditions.

Henceforth, we adopt the standard notion of thermalization from Refs. [5,7,27,28,33,34], requiring that not only the time-averaged but also the instantaneous expectation values in (1) must be close to A_{mc} for the vast majority of all sufficiently large times t, i.e., after initial transients have died out. Note that a small fraction of exceptional times t is unavoidable, e.g., due to quantum revivals, caused by the quasiperiodicity of A_t in (2). In addition to $A_\psi \simeq A_{\mathrm{mc}}$, we thus require that

$$\overline{(\langle\psi|A_t|\psi\rangle - A_\psi)^2} \ll 1. \tag{5}$$

As demonstrated, e.g., in Refs. [33–38], an arbitrary $|\psi\rangle \in \mathcal{H}$ satisfies (5) under the sufficient condition

$$S_\psi := \sum_{n=1}^{N} |\langle n|\psi\rangle|^4 \ll 1, \tag{6}$$

where we tacitly restricted ourselves to the generic case [7,27,33,34] that the energy differences $E_m - E_n$ are finite and mutually different for all pairs $m \neq n$ (generalizations are possible [35–38] but omitted here for the sake of simplicity). We thus can conclude that the sETH together with (6) are sufficient conditions for thermalization.

On the other hand, we will later provide examples which exhibit thermalization but violate the sETH. Altogether, the sETH alone is thus neither sufficient nor necessary for thermalization: We have to modify or supplement the sETH criterion, or we have to admit exceptions and show that they are "rare" in some suitable sense. In the following, we work out an approach along these lines.

To begin with, we note that the original Hilbert space of the system is usually much larger than the energy shell $\mathcal{H}$ and that A and H are *a priori* operators on that larger space. Accordingly, $I_{\mathcal{H}} := \sum_{n=1}^{N} |n\rangle\langle n|$ may also be considered as a projector onto $\mathcal{H}$ and $A' := I_{\mathcal{H}} A I_{\mathcal{H}}$ as the restriction or projection of A onto $\mathcal{H}$ (and likewise for H). But since only vectors $|\psi\rangle$ with support in $\mathcal{H}$ are considered in (1), one readily sees that every single term in (1)–(6) remains exactly the same if we replace A by A'. In particular, $A_{nn} = A'_{nn}$ for all $n \in \{1, \ldots, N\}$. On the other hand, the eigenvalues and eigenvectors of A', henceforth denoted as a_n and $|\varphi_n\rangle$, respectively, are, in general, different from those of A. From now on, we always work with A', but—for the sake of convenience and since it actually does not matter in most formulas—we again omit the prime symbol.

Possibly after adding a trivial constant to the observable and multiplying it by a constant factor, we can and will assume that

$$\mathrm{Tr}\{A\} = 0, \tag{7}$$

$$\|A\| = 1, \tag{8}$$

where $\mathrm{Tr}\{\cdot\}$ is the trace in $\mathcal{H}$ and $\|\cdot\|$ the operator norm. It follows that $a_{\max} := \max_n a_n > 0$ and $a_{\min} := \min_n a_n < 0$. For an arbitrary but fixed $a \in (0, a_{\max})$, we define

$$g(x) := \frac{1}{N} \sum_{n=1}^{N} \frac{1}{1 + x(a - a_n)}. \tag{9}$$

One readily verifies that $g(0) = 1$, $g'(0) = -a < 0$, $g(x) \to \infty$ as x approaches $x_{\max} := 1/(a_{\max} - a)$ from below, and $g''(x) > 0$ for all $x \in [0, x_{\max})$. These properties imply that there must be exactly one $x \in (0, x_{\max})$ with $g(x) = 1$. This x value is henceforth denoted as $y(a)$. One thus can conclude that $y(a) > 0$, that

$$p_n := \frac{1}{N} \frac{1}{1 + y(a)(a - a_n)} > 0 \tag{10}$$

for all $n = 1, \ldots, N$, and that

$$\sum_{n=1}^{N} p_n = 1. \tag{11}$$

Similarly, for $a \in (a_{\min}, 0)$ there is a unique $y(a) < 0$ which satisfies (10) and (11), while $y(a)$ must be zero for $a = 0$. Finally, one can deduce from (10) and (11) by means of a straightforward calculation [39] that

$$\sum_{n=1}^{N} a_n p_n = a \tag{12}$$

for any given $a \in (a_{\min}, a_{\max})$.

Next, we introduce an ensemble of random vectors $|\chi\rangle \in \mathcal{H}$ via

$$|\chi\rangle = \sum_{n=1}^{N} c_n |\chi_n\rangle, \tag{13}$$

where $\{|\chi_n\rangle\}_{n=1}^{N}$ is any orthonormal basis of $\mathcal{H}$ and where the real and imaginary parts of the c_n's are independent, Gaussian-distributed random variables of mean zero and variance $1/2N$. Denoting averages over the c_n's by $[\ldots]_c$, it follows that $[c_m^* c_n]_c = \delta_{mn}/N$ for all $m, n \in \{1, \ldots, N\}$. The random vectors (13) are thus normalized on the average, $[\langle\chi|\chi\rangle]_c = 1$, but not individually. Moreover, the random vector ensemble is invariant under arbitrary unitary transformations of the basis $\{|\chi_n\rangle\}_{n=1}^{N}$ (all its statistical properties remain unchanged). All bases are thus equivalent and the ensemble is unbiased. In terms of this ensemble, yet another ensemble of random vectors $|\phi\rangle$ is defined via

$$|\phi\rangle := \sqrt{N}\rho^{1/2}|\chi\rangle, \tag{14}$$

$$\rho := \sum_{n=1}^{N} p_n |\varphi_n\rangle\langle\varphi_n|, \tag{15}$$

where the $|\varphi_n\rangle$ have been introduced above (7) and where $\rho^{1/2} := \sum_{n=1}^{N} \sqrt{p_n}\,|\varphi_n\rangle\langle\varphi_n|$, implying $(\rho^{1/2})^2 = \rho$. Note that ρ is Hermitian, positive [see (10)], and of unit trace [see (11)], i.e., a well-defined density operator.

Given any Hermitian operator $B : \mathcal{H} \to \mathcal{H}$, one readily can infer from (13)–(15) that [40]

$$\mu_B := [\langle\phi|B|\phi\rangle]_c = \mathrm{Tr}\{\rho B\}, \tag{16}$$

$$\sigma_B^2 := [(\langle\phi|B|\phi\rangle - \mu_B)^2]_c = \mathrm{Tr}\{(\rho B)^2\}. \tag{17}$$

Taking advantage of the Cauchy-Schwarz inequality [41], $\mathrm{Tr}\{(\rho B)^2\}$ can be upper bounded by $\mathrm{Tr}\{\rho^2 B^2\}$. Evaluating the trace by means of the eigenbasis of B, one thus obtains

$$\sigma_B^2 \leq \|B\|^2 \mathrm{Tr}\{\rho^2\}. \tag{18}$$

In the following, we restrict ourselves to the case

$$d_{\mathrm{eff}} := 1/\mathrm{Tr}\{\rho^2\} \gg 1. \tag{19}$$

As observed in Ref. [34], the effective dimension d_{eff} tells us how many pure states contribute appreciably to the mixture ρ. Indeed, one readily finds—similarly as in Ref. [40]—that $[|\phi\rangle\langle\phi|]_c = \rho$. Moreover, if $p_n = 1/M$ for M of the weights p_n in (15), then $d_{\mathrm{eff}} = M$, and the $|\phi\rangle$ in (14) arise by unbiased sampling of vectors within an M-dimensional subspace of $\mathcal{H}$. In other words, d_{eff} quantifies the "diversity" of random vectors $|\phi\rangle$ contributing to ρ, and (19) ensures that the ensemble of random vectors in (14) is not "too small." Moreover, it is reasonable to expect that, unless a is very close to $a_{\max}$ or $a_{\min}$, many p_n's will notably contribute in (12), and hence the effective dimension of ρ will be large. This expectation is quantitatively confirmed in Supplemental Material [42], showing that d_{eff} is, in fact, exponentially large in the system's degrees of freedom under quite general conditions.

For $B = I_{\mathcal{H}}$, it follows from (16)–(19) that $[\langle\phi|\phi\rangle]_c = 1$ and $[(\langle\phi|\phi\rangle - 1)^2]_c \ll 1$. The vast majority of all $|\phi\rangle$ in (14) thus exhibit norms very close to unity. Next, by choosing $B = A$, it follows with (12), (15), and (16) that $\mu_A = a$ and with (8) and (17)–(19) that $\sigma_A^2 \ll 1$. The vast majority of all $|\phi\rangle$ in (14) thus exhibit expectation values $\langle\phi|A|\phi\rangle$ very close to the preset value a. Likewise, by choosing $B = \overline{A_t}$ and observing that $\|\overline{A_t}\| \leq \|A\|$, one can infer from (8) and (17)–(19) that the vast majority of all $|\phi\rangle$ in (14) yield time-averaged expectation values A_ϕ in (4) very close to $\mathrm{Tr}\{\rho\overline{A_t}\}$. Finally, one can show by similar calculations as in Ref. [40] that S_ϕ from (6) satisfies $[S_\phi]_c \leq 2/d_{\mathrm{eff}}$. Observing (19) and $S_\phi \geq 0$, it follows that S_ϕ must be very small for most $|\phi\rangle$'s from (14).

So far, the initial states $|\phi\rangle$ in (14) are, in general, not normalized. But, as seen above, the vast majority among them are almost of unit length. Hence, if we replace for every given $|\chi\rangle$ the concomitant $|\phi\rangle$ in (14) by its strictly normalized counterpart

$$|\psi\rangle := \langle\chi|\rho|\chi\rangle^{-1/2}\rho^{1/2}|\chi\rangle, \tag{20}$$

then the "new" expectation values $\langle\psi|A|\psi\rangle$ and $\langle\psi|\overline{A_t}|\psi\rangle$ will mostly remain very close to the "old" ones, i.e., to $\langle\phi|A|\phi\rangle$ and $\langle\phi|\overline{A_t}|\phi\rangle$, respectively. Likewise, S_ψ must remain very small for most $|\psi\rangle$'s. More precisely, one can show [42] that a vector $|\psi\rangle$, randomly sampled according to (13) and (20), satisfies simultaneously the three conditions $|\langle\psi|A|\psi\rangle - a| \leq 2\delta$, $|\langle\psi|\overline{A_t}|\psi\rangle - \mathrm{Tr}\{\rho\overline{A_t}\}| \leq 2\delta$, and $S_\psi \leq 4\delta$ with probability $P \geq 1\text{–}6\delta$, where $\delta := d_{\mathrm{eff}}^{-1/3}$ is exponentially small in the system's degrees of freedom.

In conclusion, the vast majority of all initial states $|\psi(0)\rangle := |\psi\rangle$ from (20) exhibit initial expectation values $\langle\psi(0)|A|\psi(0)\rangle$ very close to the preset value a in (9) and (10), and the time average in (4) satisfies very well the approximation

$$A_\psi = \mathrm{Tr}\{\rho\overline{A_t}\}. \tag{21}$$

In other words, the long time limit (4) is for most $|\psi\rangle$ very close to one and the same value, given by the right-hand side of (21). As discussed below (4), we furthermore require as a necessary condition for thermalization that those very similar long time averages of most $|\psi\rangle$'s must be close to the microcanonical expectation value A_{mc}. Exploiting (3) to infer $A_{\mathrm{mc}} = \mathrm{Tr}\{\rho_{\mathrm{mc}}\overline{A_t}\}$ [43], it follows that the right-hand side of (21) must satisfy

$$\mathrm{Tr}\{\rho\overline{A_t}\} = \mathrm{Tr}\{\rho_{\mathrm{mc}}\overline{A_t}\} \tag{22}$$

in a very good approximation. Recalling that under the same premise (19) most $|\psi\rangle$'s also satisfy (6), we can conclude that (19) and (22) are sufficient to guarantee that most $|\psi\rangle$'s from (20) exhibit thermalization.

The main feature of the random vector ensemble (20) is that the expectation value $\langle\psi|A|\psi\rangle$ is *almost* equal to a for *most* $|\psi\rangle$'s. As can be inferred from Ref. [15], this ensemble yields results for the statistics (mean and variance) of A_ψ and S_ψ which are very similar to those for an ensemble, where *all* normalized vectors, whose expectation value is *strictly* equal to a, are realized with equal probability (and all other vectors are excluded). We thus can conclude that most initial states $|\psi\rangle \in \mathcal{H}$ with $\langle\psi|A|\psi\rangle = a$ exhibit thermalization, provided (19) and (22) are fulfilled.

In principle, the observable A and the value of a uniquely determine $y(a)$ in (10) and (11). Hence, ρ in (15) follows and condition (22) can be checked. In practice, a general, explicit solution of all the necessary equations seems not possible. We thus content ourselves with a series expansion in powers of a. Since $y(0) = 0$ [see below (11)], we can expand $y(a)$ as $y'(0)a + y''(0)a^2/2 + \cdots$ and the denominator in (10) as a geometric series. Substituting all this into (11) and comparing terms with equal powers of a yields equations for $y'(0), y''(0), \ldots$ which can be iteratively solved. As a result, Eq. (15) assumes the form

$$\rho = \rho_{\mathrm{mc}} + \frac{1}{N}\sum_{k=1}^{\infty}[y(a)(A-a)]^k, \tag{23}$$

$$y(a) = (1/m_2)a - (m_3/m_2^3)a^2 + \mathcal{O}(a^3), \tag{24}$$

$$m_k := \frac{1}{N}\sum_{n=1}^{N}(a_n)^k = \mathrm{Tr}\{\rho_{\mathrm{mc}}A^k\}. \tag{25}$$

Taking into account Eq. (3), this finally yields

$$\mathrm{Tr}\{\rho\overline{A_t}\} - \mathrm{Tr}\{\rho_{\mathrm{mc}}\overline{A_t}\} = a\sum_{n=1}^{N}\frac{(A_{nn})^2}{m_2 N} + \mathcal{O}(a^2). \tag{26}$$

In view of the approximation (22), the coefficients on the right-hand side of (26) must be zero (or very small) separately for every power of a. Together with (25), we thus can conclude that

$$\frac{1}{N}\sum_{n=1}^{N}(A_{nn})^2 \ll \mathrm{Tr}\{\rho_{\mathrm{mc}}A^2\} \leq 1, \tag{27}$$

where we utilized (8) in the last step. This is the main result of this Letter. It implies that *most* A_{nn}'s must be very small [43]. In other words, the values of $\langle n|A|n\rangle$ must be very similar to each other for most energy eigenvectors $|n\rangle$ with eigenvalues E_n in the considered energy interval $[E-\epsilon, E]$. Following Refs. [16–20], the latter property is denoted as the *weak ETH* (wETH). In Ref. [11], somewhat similar results have been obtained for some particular initial (mixed) states which arise by certain very small perturbation of a canonical density operator [44].

In short, we found that typicality of thermalization implies the wETH. In the opposite case, i.e., when most $|\psi\rangle$'s do not exhibit thermalization, then most of them still approach very similar long time averages according to (21). However, (22) is no longer fulfilled; hence, the right-hand side of (26) is non-negligible and the wETH is violated. In other words, the wETH implies typicality of thermalization. As announced below (6), a system which violates the sETH thus exhibits thermalization provided it still satisfies the wETH. Moreover, it is noteworthy that—at least for not too large a values—the typical deviation from the thermal expectation value $A_{\mathrm{mc}} = \mathrm{Tr}\{\rho_{\mathrm{mc}}\overline{A_t}\} = 0$ [43] in (26) exhibits the same sign as the initial expectation value $\langle\psi|A|\psi\rangle = a$ itself.

Clearly, in all those conclusions, Eq. (26) plays a pivotal role, connecting the decisive quantity for thermalization (left-hand side) with the essential quantifier of the wETH (sum on the right-hand side). Our above line of reasoning thus has the virtue of being concise and "natural." Its shortcoming is that the arguments are not mathematically rigorous. [In fact, already the convergence of the expansions in (23) and (24) may strictly speaking be questionable.] A complementary, more rigorous but less enlightening line of reasoning is provided as Supplemental Material [42].

In conclusion, the weak ETH has been established as a necessary and sufficient prerequisite for thermalization in isolated many-body quantum systems in the following sense: The vast majority of all pure states, which exhibit the same initial expectation value for some observable A, closely approach the pertinent microcanonical expectation value of A for practically all sufficiently large times. It is remarkable that also in several other related studies it is the weak rather than the strong ETH which naturally arises [11,24,26,45]. Note that the necessity of the (weak or strong) ETH for thermalization is not something that one might have expected *a priori* due to some intuitively quite obvious reasons [2,9]. For instance, Peres argues [46] that generic (chaotic) systems should entail pseudorandom A_{nn}'s, which are statistically independent of the $|\langle n|\psi\rangle|^2$ in (4) for most $|\psi\rangle$. If this quite reasonable-looking expectation was correct, then the right-hand side of (4) could be well approximated by $\mathrm{Tr}\{\rho_{\mathrm{mc}}A\}$, implying

thermalization even if the (weak or strong) ETH were violated. In contrast, our key relation (26) shows that the $|\langle n|\psi\rangle|^2$ and the A_{nn} in (4) must be "correlated" in a very subtle manner, except for the "trivial case" that most of the A_{nn}'s are very similar to each other, i.e., unless A satisfies the weak ETH in the first place. Put differently, whenever typical nonequilibrium initial states do not exhibit thermalization, then such correlations must be a generic feature. Indeed, they can be seen in numerical examples [6], but their intuitive physical origin previously appeared to be a mystery to the present author. Our dynamical typicality approach provides at least a first step towards its resolution: In order to exhibit any nonthermal expectation value, most initial states $|\psi\rangle$ in (20) must necessarily acquire some sort of "correlation" with A via (10) and (15).

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[39] Equation (10) implies $\sum_{n=1}^{N}[1+y(a)(a-a_n)]p_n=1$. With (11), this yields $1+y(a)[a-\sum_{n=1}^{N}a_np_n]=1$ and thus (12) if $y(a)\neq 0$. If $y(a)=0$, we recover (12) by observing (7), (10), and $a=0$ [see below (11)].

[40] Equations (13) and (14) imply $\mu_B=\sum_{m,n=1}^{N}[c_m^*c_n]_c\langle\chi_m|B'|\chi_n\rangle$, where μ_B is defined in (16) and $B'\coloneqq\rho^{1/2}B\rho^{1/2}$. Since $[c_m^*c_n]_c=\delta_{mn}/N$ [see below (13)], we obtain $\mu_B=\mathrm{Tr}\{B'\}=\mathrm{Tr}\{\rho^{1/2}B\rho^{1/2}\}=\mathrm{Tr}\{\rho B\}$, proving (16). Upon verifying and exploiting that $[c_j^*c_kc_m^*c_n]_c=(\delta_{jk}\delta_{mn}+\delta_{jn}\delta_{\mathrm{km}})/N^2$, a similar calculation yields (17).

[41] Viewing $\mathrm{Tr}\{C^\dagger D\}$ as a scalar product, the Cauchy-Schwarz inequality reads $|\mathrm{Tr}\{C^\dagger D\}|^2\leq\mathrm{Tr}\{C^\dagger C\}\mathrm{Tr}\{D^\dagger D\}$. Choosing $C=B\rho$ and $D=\rho B$ yields $\mathrm{Tr}\{C^\dagger C\}=\mathrm{Tr}\{D^\dagger D\}=\mathrm{Tr}\{\rho^2B^2\}$ and thus $\mathrm{Tr}\{(\rho B)^2\}=\mathrm{Tr}\{C^\dagger D\}\leq\mathrm{Tr}\{\rho^2B^2\}$.

[42] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.120.230601 for mathematical details.

[43] Because of (7), $A_{\mathrm{mc}}\coloneqq\mathrm{Tr}\{\rho_{\mathrm{mc}}A\}=\mathrm{Tr}\{\rho_{\mathrm{mc}}\overline{A_t}\}$ happens to vanish, but, for the sake of formal clarity, we keep writing A_{mc} and $\mathrm{Tr}\{\rho_{\mathrm{mc}}\overline{A_t}\}$, e.g., in (22) and (26). For the same reason, the average of the A_{nn}'s (over all $n=1,\ldots,N$) happens to be zero.

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