Total correlations of the diagonal ensemble as a generic indicator for ergodicity breaking in quantum systems

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(Received 15 November 2016; revised manuscript received 30 January 2017; published 14 March 2017)

The diagonal ensemble is the infinite time average of a quantum state following unitary dynamics in systems without degeneracies. In analogy to the time average of a classical phase-space dynamics, it is intimately related to the ergodic properties of the quantum system giving information on the spreading of the initial state in the eigenstates of the Hamiltonian. In this work we apply a concept from quantum information, known as total correlations, to the diagonal ensemble. Forming an upper bound on the multipartite entanglement, it quantifies the combination of both classical and quantum correlations in a mixed state. We generalize the total correlations of the diagonal ensemble to more general α-Renyi entropies and focus on the cases $\alpha = 1$ and $\alpha = 2$ with further numerical extensions in mind. Here we show that the total correlations of the diagonal ensemble is a generic indicator of ergodicity breaking, displaying a subextensive behavior when the system is ergodic. We demonstrate this by investigating its scaling in a range of spin chain models focusing not only on the cases of integrability breaking but also emphasize its role in understanding the transition from an ergodic to a many-body localized phase in systems with disorder or quasiperiodicity.

DOI: 10.1103/PhysRevB.95.125118

I. INTRODUCTION

Attempts to recover statistical mechanics from the underlying unitary dynamics of a quantum system have been around since the inception of quantum theory with the pioneering approaches of both von Neumann [1] and Schrödinger [2]. Although these works showed impressive foresight, until relatively recently these foundational studies were almost forgotten and seen as irrelevant due to the fact that unitary evolution was not relevant over dynamical time scales in the laboratory. Arguments for the validity of statistical mechanics predominantly consisted of invoking coupling to the larger bath of the universe and hence thermalization by dissipation.

In the past two decades, these foundational questions have seen an unprecedented resurgence in interest by theorists from several different scientific communities, ranging from condensed matter physics to quantum information [3–10]. This revival is due, in no small part, to great advances in experimental ultracold atomic physics [11] where pioneering experiments were successful in generating and probing coherent unitary dynamics over long time scales [12–15]. This includes an experimental realization [13] of the Lieb-Liniger model of interacting bosons in one dimension, in which the existence of an extensive set of conserved quantities, due to the integrability of the model, renders the dynamics nonergodic [16].

Experimental motivations aside, there have also been developments in theoretical condensed matter physics, which have forced us to carefully think about the foundations of statistical mechanics beyond the paradigm of integrable systems. In particular Basko, Aleiner, and Altshuler have demonstrated that Anderson localization [17] is stable in the presence of interactions [18] leading to a new type of transition to a phase, which is known as many-body localization (MBL) [19–21]. Interestingly this transition is between an ergodic and a nonergodic phase [22] and has led to an intense interest in the phenomenology of ergodicity and its breaking in quantum dynamics.

Physically motivated, an approach known as the eigenstate thermalization hypothesis (ETH) has proven to be popular among researchers from this community. The ETH was born out of a realization by Berry [23], who postulated that, in the semiclassical limit of quantum systems with chaotic classical counterparts, the Wigner function evaluated on eigenstates reduces to the microcanonical distribution. This was extended to arbitrary systems by Deutsch [24], who proposed to assume that generic eigenstates of ergodic systems are like eigenstates of full random matrices. Building on these ideas Srednicki formulated what is now known as the ETH, which is an ansatz on the behavior of matrix elements of observables with the consequence that ergodic systems can show thermal behavior at the level of individual eigenstates [25–27].

Another approach, popular in the quantum information and mathematical physics communities, is the concept of normal and canonical typicality [28–32]. This approach has the advantage of not just replacing one hypothesis (that systems tend to equilibrate to Gibbs states) with another equally unproven one (that systems generically fulfill the ETH), but it replaces the equal *a priori* probability postulate (all states in a microcanonical shell are equally probable) with a strictly weaker assumption, by showing rigorously that the overwhelming majority of states in a microcanonical shell have nearly the same properties with respect to certain observables, such as, for example, local ones. However, the generality of the results obtained based on these concepts makes it difficult to apply this approach to concrete systems, as in realistic

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situations interesting dynamics usually starts from a highly untypical initial condition.

In addition to the above, in recent years dynamical equilibration of expectation values and density matrices of subsystems under unitary dynamics has been studied extensively [32–37] (see also Ref. [8] for a review). Such equilibration can be rigorously shown to happen if the spectrum of the Hamiltonian fulfills certain nonresonance conditions, and the initial state has overlap with many energy eigenstates or the second most populated eigenstates are occupied with only a small probability (a weaker requirement). In these results, the equilibrium expectation values or reduced states are given by the diagonal ensemble (also known as infinite time averaged state, dephased state, or pinched state). How and to which state equilibration occurs, of course, is closely connected to whether a system is ergodic or not, which motivates us to consider in more detail the correlations in this diagonal ensemble to study ergodicity breaking.

Concepts of quantum information have been useful in the typicality approach (system-bath entanglement) [30], the dynamical equilibration approach, and in the ETH approach; for example, in studying the volume law scaling of entanglement in eigenstates, the crossover to an area law is a signature of the MBL transition [38]. In a recent work, some of the current authors have proposed a different information-theory-inspired approach [39]. The idea is to look at the correlations within the diagonal ensemble to understand nonergodic behavior in the context of the MBL transition [39]. The purpose of the current work is to demonstrate that this concept is more generally useful and can detect ergodicity breaking in a range of scenarios beyond and including MBL. The formalism offers a fresh approach to ergodicity and its breaking in quantum systems, while at the same time giving us novel insights into the structure of correlations in the equilibrium state of dynamical systems.

II. ERGODICITY AND TOTAL CORRELATIONS

Due to the absence of a universally valid phase-space picture in quantum systems it is not obvious how to generalize the concept of ergodicity to the quantum realm, especially in systems that do not have a well-defined classical limit. As was outlined in Ref. [39], the total correlations in the diagonal ensemble offer a physically meaningful way to define and probe ergodicity and its breaking in quantum systems. Here we generalize this approach.

A. A condition for ergodicity

The (quasi)ergodic hypothesis in classical systems states that over time a system's dynamics uniformly covers its entire phase space so that the (infinite time) time average and the microcanonical averages agree [40]. It is thus natural to define ergodicity in quantum systems in an analogous way via the portion of the explored Hilbert space. A complication is that quantum systems explore all of the available phase space uniformly such that time and microcanonical average agree exactly only for very special initial states. This naturally leads us to build a notion of ergodicity in quantum systems based on the fraction of the available Hilbert space that is explored, as opposed to the classical notion of ergodicity that requires that all of the available phase space is explored uniformly. The available Hilbert space hereby can be usually naturally defined as, for example, the fixed magnetization or fixed filling fraction subspace if the system has such symmetries. To define ergodicity via the fraction of Hilbert space that is explored one obviously first needs to devise a way of quantifying the explored fraction. It is this question that we elucidate in this work, going beyond the initial proposal in Ref. [39].

For a fixed initial state ρ and nondegenerate Hamiltonian H the diagonal ensemble is defined as

$$\omega := \sum_n |E_n\rangle\langle E_n|\,\rho\,|E_n\rangle\langle E_n| = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt\, e^{-itH}\,\rho\, e^{itH}, \tag{1}$$

where $|E_n\rangle$ are the eigenvectors of H. The state ω is the state that maximizes the von Neumann entropy subject to all constants of motion [41]. For pure initial states $\rho = |\Psi\rangle\langle\Psi|$, the inverse purity $1/\mathrm{tr}(\omega^2)$ of the diagonal ensemble can be seen as a measure for how spread out the initial state was over the different eigenstates of the Hamiltonian and it often goes under the apt name of effective dimension or participation ratio. If the effective dimension is high, expectation values of observables can be rigorously shown [4,6,8,32,33] to equilibrate on average during the time evolution towards their values in the state ω. The effective dimension, however, is not the only way of quantifying the spreading of the initial state. Another measure is the von Neumann entropy of the diagonal ensemble $S(\omega) = -\sum_n p_n \log_2 p_n$ with $p_n = |\langle E_n|\Psi\rangle|^2$ and derived quantities; this was the route taken in Ref. [39].

Both of these quantities are special cases of a whole family of entropies, the so-called α-Renyi entropies, which for $0 < \alpha < \infty$ are defined as

$$S_\alpha(\rho) := \frac{1}{1-\alpha}\log_2[\mathrm{tr}(\rho^\alpha)]. \tag{2}$$

The 2-entropy $S_2 = \log_2[1/\mathrm{tr}(\rho^2)]$ is the log of the inverse purity, the 1-entropy $S_1 = S$ is the von Neumann entropy, and the two extreme cases are defined as $S_\infty(\rho) := \log_2(1/\|\rho\|_\infty)$ and $S_0(\rho) := \log_2[\mathrm{rank}(\rho)]$. The Renyi entropies are monotonically nonincreasing as a function of α. In other words, for any fixed ρ, it holds that $S_\alpha(\rho) \leqslant S_{\alpha'}(\rho)$ whenever $\alpha' \geqslant \alpha$. For ψ a pure state and ρ a normalized quantum state of a system with Hilbert space dimension d, it holds that

$$0 = S_\alpha(\psi) \leqslant S_\alpha(\rho) \leqslant S_\alpha(\mathbb{1}_{d\times d}/d) = \log_2(d). \tag{3}$$

Except in the case $\alpha = 0$ the inequalities hold with equality only if ρ is either pure or maximally mixed, respectively.

It is the upper bound that interests us here. Given a Hamiltonian H, an initial state ρ explores all of Hilbert space if $S_\alpha(\omega) = \log_2(d)$. As said above, this, however, only happens for very special states for which ω is maximally mixed. A natural relaxation of this condition is to demand that for some chosen $0 \leqslant \alpha \leqslant \infty$ there exists a constant $\lambda > 0$, independent of N and d, such that $S_\alpha(\omega) \geqslant \log_2(\lambda\, d)$, i.e., that the state explores a λ fraction of the Hilbert space as measured by the α-Renyi entropy.

That this is a sensible condition for ergodicity is further illustrated by the following consideration: For any fixed initial state ρ and Hamiltonians H with eigenbasis randomly drawn from a unitary invariant ensemble on a Hilbert space of dimension d one can show for the $\alpha = 1$ entropy [Ref. [42], Eq. (B6)] and the $\alpha = 2$ entropy [33] that the probability that the state explores less than half of the available Hilbert space is at least almost exponentially suppressed with growing d (as the Renyi entropies are nonincreasing as a function of α this then holds for all $0 \leqslant \alpha \leqslant 2$). That is, any fixed initial state is with high probability ergodic according to our condition with respect to Hamiltonians drawn unitarily at random—as one would expect. To be more precise: Generalizing the considerations from Ref. [39] we hence demand that a system should be considered α ergodic only if the initial states explore at least a constant fraction of the available Hilbert space in the sense that for some λ it holds that $S_\alpha(\omega) \geqslant \log_2(\lambda\, d)$. In the models that we will consider the Neel states are suitable initial states.

We have so far defined a family of conditions parametrized by α that appear as natural quantum generalizations of the concept of ergodicity, but have not yet said much about the role of α. Remember that the Renyi entropies are monotonically nonincreasing as a function of α. Thus, demanding that, for example, $S_2 \geqslant \log_2(\lambda\, d)$ is a stronger requirement than demanding that the same scaling holds for S_1. As we will see later, the fact that a system fulfills our condition for ergodicity for a given α has direct consequences on the scaling of the total correlations with the number of particles.

B. Total correlations

Phase transitions that involve the breaking of ergodicity, such as the MBL transition, have in the past been analyzed with various measures of correlations. A focus thereby was on the mutual information, which was found to saturate to a constant in Anderson localization, grow logarithmically in time in the MBL phase, and linearly in ergodic phases [43]. Further, it decays exponentially with the distance between subsystems in the localized phase, but slower than exponentially in the ergodic phase. Here we concentrate on a correlation measure called the total correlations and its Renyi generalizations.

Concretely we define the α-Renyi total correlations as

$$T_\alpha(\rho) := \sum_{m=1}^{N} S_\alpha(\rho_m) - S_\alpha(\rho), \tag{4}$$

where ρ_m is the marginal (reduced state) of ρ on site m. In the special case $\alpha = 1$ the total correlations have the following operational meaning: Let $\mathcal{P}$ be the set of all product states of an N-partite quantum system, i.e., for spin systems, states of the form $\pi = \pi_1 \otimes \pi_2 \cdots \otimes \pi_N$, and the obvious analogs for fermionic and bosonic systems, then [44]

$$T_1(\rho) = \min_{\pi \in \mathcal{P}} S(\rho \| \pi), \tag{5}$$

where $S(\rho\|\sigma) := -\mathrm{tr}(\rho \log_2 \sigma) - S_1(\rho)$ is the relative entropy between the states ρ and σ and it can be thought of as a measure of distinguishability of the two states. More precisely, the relative entropy quantifies how difficult it is to distinguish between many copies of ρ and many copies of σ in a hypothesis testing scenario [45]. It turns out that there is a unique product state that minimizes the relative entropy in the above expression and this is the product of the reduced states ρ_m of ρ, i.e., $\pi = \otimes_{m=1}^{N} \rho_m$ [44]. In the case $\alpha = 1$ the total correlations can hence be thought of as the distinguishability from the closest product state. No such straightforward operational interpretation exists for $\alpha \neq 1$ to the best of our knowledge. As we will explain in the next sections, insights into integrability breaking can be obtained through the various Renyi total correlations.

C. Scaling of the total correlations

In the following we analyze the total correlations, and in particular T_1 and T_2, of the diagonal ensemble ω for Neel initial states in various spin-chain models. One characteristic that will be very insightful is the scaling of the total correlations with N.

Inspecting Eq. (4) one might expect that the total correlations $T(\omega)$ in the diagonal ensemble should generally scale extensively in the system size N, i.e., for large N, to leading order, it should scale like

$$T_\alpha(\omega) \propto N, \tag{6}$$

as $T_\alpha(\omega)$ involves the sum $\sum_{m=1}^{N} S_\alpha(\omega_m)$ of the N subsystem entropies.

If a family of systems of increasing size satisfies the condition for ergodicity defined above, then the contribution linear in N from the first sum can be precisely canceled by the $-S_\alpha(\omega)$ term; $S_\alpha(\omega)$ is known as the diagonal entropy [46] and is a measure of localization in the energy eigenbasis. Consider a quantum spin chain of local dimension 2 in the zero magnetization subspace.[1] The available Hilbert space dimension is $d = \binom{N}{N/2} = N!/(\frac{N}{2}!)^2 \geqslant \sqrt{8\pi}\, \mathrm{e}^{-2}\, 2^N/\sqrt{N}$ and $S_\alpha(\omega_m) \leqslant \log_2 2 = 1$, so that if the condition for ergodicity $S_\alpha(\omega) \geqslant \log_2(\lambda\, d)$ holds, one finds at most the logarithmic scaling

$$T_\alpha(\omega) \leqslant \log_2(N)/2 - \log_2(\lambda \sqrt{8\pi}\, \mathrm{e}^{-2}). \tag{7}$$

One furthermore retains a logarithmic scaling for ergodic systems for all other constant magnetization/fillings subspaces $\eta \neq 1/2$ in the case $\alpha = 1$ [39].

This subextensive scaling can also be understood intuitively: The transport present in ergodic systems correlates the different parts of the system to the extent that they appear, for most times during the evolution, so mixed that the time-averaged state starts to resemble a product state.

In conclusion we can say that whenever we see a faster than logarithmic scaling in the α-Renyi total correlations of the diagonal ensembles ω of an initial state from the half-filling subspace, then the condition for ergodicity for that value of α is violated. On the contrary, a logarithmic scaling suggests ergodic behavior.

[1] The diagonal entropy, or Shannon entropy in the energy eigenbasis, measures delocalization/localization in that basis and therefore its scaling can give information about ergodicity. However, the total correlations and its Renyi generalizations give far more information; in particular it not only scales differently in different phases but also shows divergence of the correlations in the critical region—an interesting phenomenon in its own right, which cannot be studied just looking at the diagonal entropy alone.

III. EXAMPLES

Low-dimensional many-body quantum systems, such as spin-1/2 chains are systems commonly used to study ergodicity breaking phenomena. In what follows we will always consider dynamics starting from the trivial initial Hamiltonian, H_0 defined as

$$H_0 = \sum_{i=1}^{N} J_z s_z^i s_z^{i+1}, \tag{8}$$

where s^i are spin-1/2 operators, and we choose as an initial state the Neel state $|\Psi_0\rangle = |\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\ldots\rangle$. Now imagine a quench where we turn on additional terms denoted by an interaction part H_{int} such that dynamics is initiated and governed by the Hamiltonian $H_F = H_0 + H_{\text{int}}$. We shall build the diagonal ensemble defined by Eq. (1) by exact diagonalization and then investigate the scaling of the total correlations $T(\omega)$ as defined in Eq. (4), both in the case of the von Neumann total correlations ($\alpha = 1$) and of the 2-Renyi total correlations ($\alpha = 2$). We choose the initial state $|\Psi_0\rangle$ as a Neel state for two principal reasons: First, in the models we shall consider, the Neel state can be shown to sample eigenstates of H_F at the center of the spectrum and in the half-filling subspace [47]. In this regime we expect the finite-size effects to be minimized. Second, the Neel state (charge density wave in fermion picture), is by now routinely prepared by experimentalists to study ergodicity breaking, for example in the recent studies of MBL systems [48,49].

A. Integrability breaking

Let us begin with the following model studied by Santos in 2004 [50]. The model is an XXZ spin chain with open boundary conditions, which includes a single defect at the center of the chain of strength ϵ,

$$H_F = \sum_{i=1}^{N} \left[J_x s_x^i s_x^{i+1} + J_y s_y^i s_y^{i+1} + J_z s_z^i s_z^{i+1} \right] + \epsilon s_z^{N/2}. \tag{9}$$

The integrability of the chain is broken [50], indicated by a crossover from Poissonian to Wigner-Dyson statistics, for defect strengths which are comparable to the interaction energy. As the strength of the single defect is increased the system becomes integrable again as the chain is cut into two XXZ chains. Our theory predicts then that we should see a linear-log-linear behavior in the scaling of the total correlations as we increase the defect strength from zero. This is indeed what results from the numerical computation of $T_1(\omega)$, shown in the main plot of Fig. 1 for three values of ϵ, $\epsilon = 0$, 0.5, and 10: T_1 scales linearly for the values $\epsilon = 0$ and $\epsilon = 10$ and approximately logarithmically for $\epsilon = 0.5$ as a function of system size. The same happens to the 2-Renyi total correlations $T_2(\omega)$, shown in the main plot of Fig. 2.

The second model that we consider is the clean XXZ model with next-nearest-neighbour interaction,

$$H_{\text{NNN}} = \sum_{i=1}^{N} \left[J_x s_x^i s_x^{i+1} + J_y s_y^i s_y^{i+1} + J_z s_z^i s_z^{i+1} + J'_x s_x^i s_x^{i+2} + J'_y s_y^i s_y^{i+2} \right]. \tag{10}$$

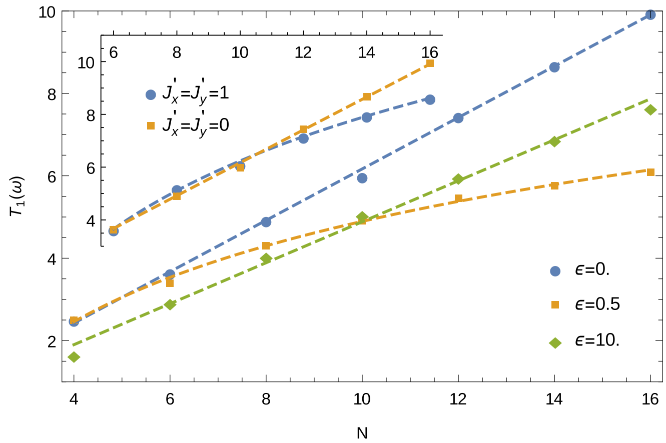

FIG. 1. The von Neumann total correlations of the diagonal ensemble starting with the Neel state for an XXZ chain with defect of strength ϵ placed at center of the chain [Eq. (9) with parameters $J_x = J_y = 1$, and $J_z = 0.5$]. When the defect strength is zero or very strong the model is integrable, which is reflected in a linear scaling of the total correlations, and when it is comparable with the interaction energy it shows a logarithmic growth indicative of ergodic dynamics. Inset: Total correlations for an XXZ chain with next-nearest-neighbour interaction [Eq. (10) with parameters $J_x = J_y = 1$, $J_z = 0.5$, and $J'_x = J'_y = 1$, compared to the same model with $J'_x = J'_y = 0$]. The model is nonintegrable and thus the scaling of the total correlations is logarithmic in the system size.

For $J'_x, J'_y \neq 0$ integrability is broken and the scaling of the total correlations $T_1(\omega)$ with the system size is logarithmic, as is shown in the inset of Fig. 1. Also in this model we see an analogous behavior for the 2-Renyi total correlations $T_2(\omega)$, which are logarithmically scaling with the system size (see

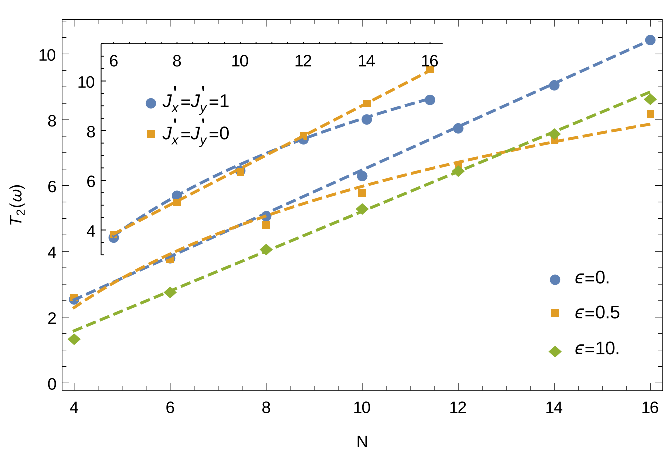

FIG. 2. The 2-Renyi total correlations of the diagonal ensemble starting with the Neel state for an XXZ chain with defect of strength ϵ placed at center of the chain [Eq. (9) with parameters $J_x = J_y = 1$, and $J_z = 0.5$]. When the defect strength is zero or very strong T_2 scales linearly with system size and when it is comparable with the interaction energy it scales logarithmically. Inset. Total correlations for an XXZ chain with next-nearest-neighbour interaction [Eq. (10) with parameters $J_x = J_y = 1$, $J_z = 0.5$, and $J'_x = J'_y = 1$, compared to the same model with $J'_x = J'_y = 0$]. The scaling of the total correlations is logarithmic in the system size.

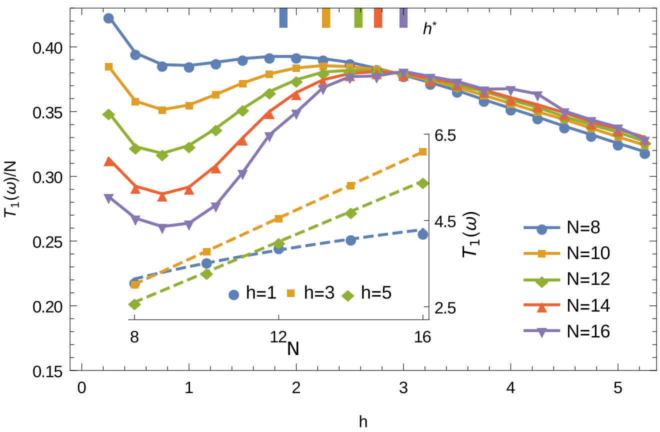

FIG. 3. The von Neumann total correlations of the diagonal ensemble, starting with a Neel state, for the Heisenberg model with random fields [whose Hamiltonian is Eq. (11) with $h_i \in [-h,h]$ and $J_x = J_y = J_z = 1$], rescaled with the system size. The markers on the top axis denote the positions of the local peak $h^*(N)$. The curves show a system-size-dependent peak (see Fig. 7) and collapse for $h \gtrsim 2.5$. Inset: System size scaling of the total correlations for three example values of h, showing a logarithmic scaling deep in the delocalized phase and a linear scaling for disorder values near the transition (which is at $h_c \approx 3.7$) and in the localized phase.

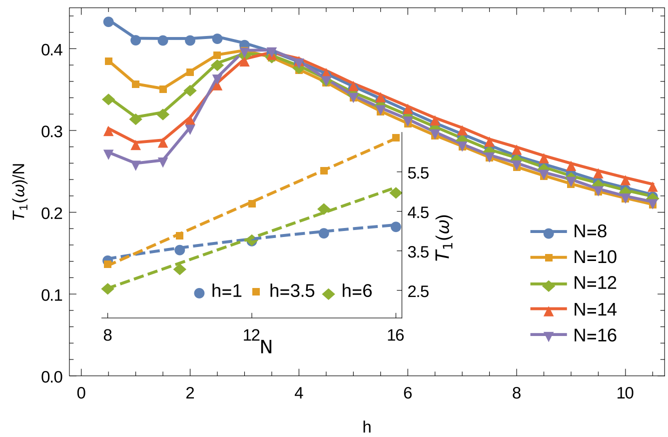

FIG. 4. The von Neumann total correlations of the diagonal ensemble, starting with a Neel state, for the Aubry-André model [whose Hamiltonian is Eq. (11) with the cosine h_i fields and $J_x = J_y = J_z = 1$], rescaled with the system size. The curves show a system-size-dependent peak and collapse for $h \gtrsim 3.5$. Inset: System size scaling of the total correlations for three example values of h, showing a logarithmic scaling deep in the delocalized phase and a linear scaling in the localized phase.

the inset of Fig. 2). In both cases of integrability breaking, the total correlations displays the predicted behavior.

B. Many-body localization

Let us now consider models that have an MBL transition that separates an ergodic phase and a nonergodic one where a sufficient number of local integrals of motion exists in order to have a breaking of the ETH [51]. We look at a system with the Hamiltonian

$$H_{\text{MBL}} = \sum_{i=1}^{N} \left[J_x s_x^i s_x^{i+1} + J_y s_y^i s_y^{i+1} + J_z s_z^i s_z^{i+1} + h_i s_z^i \right], \quad (11)$$

where $h_i \in [-h,h]$ is a disordered field (Heisenberg model with random fields) or $h_i = h\cos(2\pi\phi^{-1}i + \delta)$, where ϕ is the golden ratio and δ is a random phase in $[0,2\pi)$, that is a pseudodisordered cosine field (Aubry-André model). For both models we compute the total correlations for the diagonal ensemble with the Neel initial state, averaging over many disorder or pseudodisorder realizations, the latter obtained through the random phase δ (10^5 realizations for $N \leqslant 12$, 10^4 for $N = 14$, and 250–1000 for $N = 16$). The results for the von Neumann total correlation rescaled with the system size, $T_1(\omega)/N$, are shown in Figs. 3 and 4, respectively, for the two models, as a function of the disorder or quasidisorder strength.

We note two features: the curves collapse for $h \geqslant h^*$, indicating a linear scaling of the total correlations and thus nonergodicity, and $T_1(\omega)/N$ peaks at a value $h^*(N)$. Remarkably, the presence of a peak can be understood as a divergence of correlations at the MBL transition point and its asymptotic position in the infinite-size limit gives the transition value h_c [39]. We are able to perform such extrapolation (see Fig. 7), thus obtaining $h_c^{\text{H}} = \lim_{N\to\infty} h^{\text{H}^*} = 4.0 \pm 0.2$ for the random potential and $h_c^{\text{AA}} = \lim_{N\to\infty} h^{\text{AA}^*} = 4.5 \pm 0.9$ for the Aubry-André potential. Note that for the latter case the extrapolation suffers from much larger errors due to the smaller movement of the peak of the finite-size data with respect to its error.

For the Heisenberg model with random fields the transition value has been estimated through other numerical evidence [38,52,53] to be equal to $h_c^{\text{H}} = 3.7(2)$ at the center of the band for the parameters that we used, although its actual value could be larger ($h_c^{\text{H}} \geqslant 4.5$ according to Ref. [54]); an equivalent high-quality numerical result is not available for the Aubry-André model, although experimental works find the localization transition at similar values [48]. Interestingly, as soon as interactions are introduced, the Aubry-André model acquires almost identical features to the Heisenberg with random fields model first studied by total correlations in Ref. [39]. Finally, for both models, for weak (quasi)disorder ($h \lesssim h^*$), the scaling of the total correlations is logarithmic, implying an ergodic phase.

Let us now consider the 2-Renyi total correlations, focusing first on the Heisenberg model with random fields. The total correlations rescaled by the system size $T_2(\omega)/N$ are shown in Fig. 5, showing a collapse for $h \gtrsim 2$ for the available system sizes, to be compared with an analogous behavior of $T_1(\omega)/N$, where the collapse point is ≈ 2.5. For a system of infinite size, one would expect that the collapse points (or equivalently the peak positions) should be the same for all total correlations T_α; due to the stronger ergodicity requirement of higher-α Renyi entropies, however, it is understandable that T_2 gives an underestimation at finite, small system sizes.

As expected, T_2 scales linearly with the system size for $h \gtrsim h_2^*$ and logarithmically for $h \lesssim h_2^*$. Moreover, the curves in Fig. 5 peak on a system-size-dependent value $h_2^*(N)$. In Fig. 7 we show the scaling of the T_1 and T_2 peak positions with the

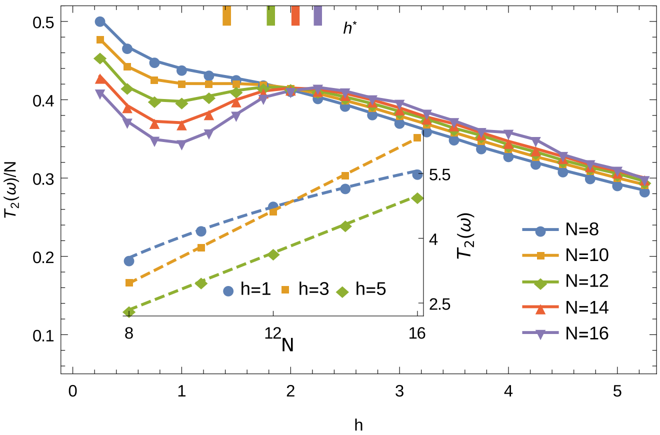

FIG. 5. The 2-Renyi total correlations of the diagonal ensemble, starting with a Neel state, for the Heisenberg model with random fields [whose Hamiltonian is Eq. (11) with $h_i \in [-h,h]$ and $J_x = J_y = J_z = 1$], rescaled with the system size. The markers on the top axis denote the positions of the local peak $h^*(N)$, excluding the case $N = 8$, where no local maximum can be discerned. The curves show a system-size-dependent peak (see Fig. 7) and collapse for $h \gtrsim 2$. Inset: System size scaling of the total correlations for three example values of h, showing a logarithmic scaling deep in the delocalized phase and a linear scaling for disorder values near the transition (which is at $h_c \approx 3.7$) and in the localized phase.

system size. For both the T_1 and T_2 peak positions, the finite-size scaling is very well approximated by a linear behavior in $1/N$; the infinite-size extrapolation for the 2-Renyi case is $h_2^*(\infty) = 3.6 \pm 0.2$, which is lower than the value obtained from the von Neumann total correlations. This is again a signal of the underestimation of the breaking of ergodicity and of stronger finite-size effects due to the hierarchy in the Renyi entropies.

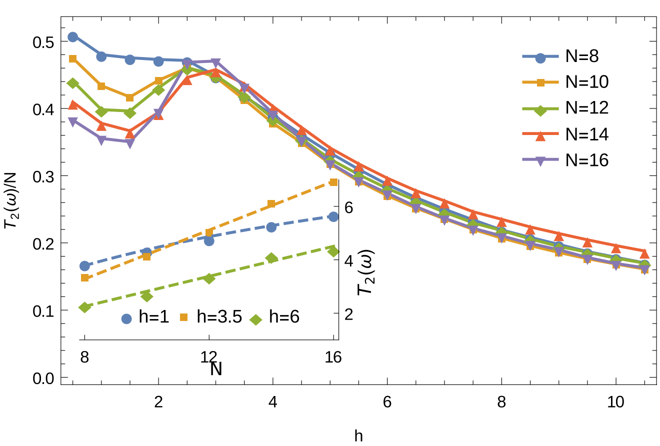

FIG. 6. The 2-Renyi total correlations of the diagonal ensemble, starting with a Neel state, for the Aubry-André model [whose Hamiltonian is Eq. (11) with the cosine h_i fields and $J_x = J_y = J_z = 1$], rescaled with the system size. The curves show a system-size-dependent peak (see Fig. 7) and collapse for $h \gtrsim 3$. Inset: System size scaling of the total correlations for three example values of h, showing a logarithmic scaling deep in the delocalized phase and a linear scaling in the localized phase.

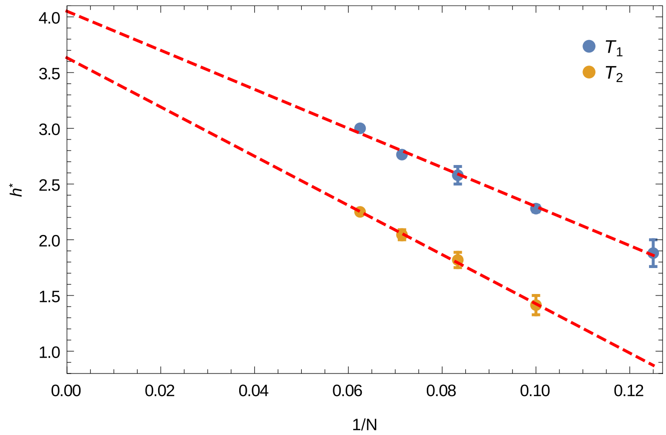

FIG. 7. System size scaling of the peak of the total correlations in the Heisenberg model with random fields, for both T_1 and T_2. The peak is extracted from a polynomial interpolation of each of the curves in Figs. 3 and 5, in which it is denoted with a marker on the top axis. We perform a linear fit in $1/N$ and obtain the infinite size extrapolation given in the text.

Finally, in Fig. 6 we show the results for the 2-Renyi total correlations of the Aubry-André model. The qualitative behavior is again the same as for the model with random fields, showing once again that the interactions remove the special integrability features of a noninteracting Aubry-André model. Specifically, $T_2(\omega)/N$ has a peak, which scales to $h_2^*(\infty) = 3.5 \pm 0.6$, which, analogously to what happens in the random fields model, is a lower value than the result for the extrapolated peak of the rescaled von Neumann total correlations.

IV. CONCLUSIONS

The results displayed in this work demonstrate that the total correlations of the diagonal ensemble is a powerful concept to understand ergodicity breaking in quantum systems in general. The numerics performed in different models confirm that the scalings predicted in the theory first outlined in Ref. [39] work in the cases of both integrability breaking and also ergodic to MBL transitions. Within the context of systems that show ergodicity breaking, a number of methods have proven useful, especially in the case of localizable systems, consisting in examining the participation ratio [55], the entanglement entropy [56], and the full entanglement spectrum [57]. The total correlations presented here are an additional tool for such systems. Where MBL systems are concerned the rescaled quantity offers the additional feature of peaking around the expected transition point; given that this may be seen as a divergence of correlations in the infinite time steady state, it represents a novel contribution to the theory of quantum correlations. The peak was observed in two models displaying a MBL transition.

We have examined the total correlations (4) for two values of α, $\alpha = 1$ and $\alpha = 2$; the 2-Renyi total correlations has the numerical advantage, being more suitable to be computed avoiding the diagonalization of the density matrix through faster techniques such as t-DMRG, where a finite time average could be performed. A topic for future research is to increase the system sizes dramatically by applying t-DMRG and finite time averaging to compute the 2-Renyi total correlations.

Finally, given the rapid progress in experimental techniques it seems possible that the total correlations could be experimentally measured in the near future. The total correlations amount to subtracting the diagonal entropy from the sum of the entropies of the marginal states. The marginal states and their entropies can already be measured in a quench starting from a Neel state [49]. Measuring the diagonal entropy is a more challenging task, however, some progress has been made in this direction for small systems [58] and given the current interest in measuring Renyi entropies in experiments [59] we believe that further advances could yield the experimental extraction of total correlations.

ACKNOWLEDGMENTS

F.P. would like to thank G. Parisi for useful discussions and SISSA and ICTP for access to computing resources and hospitality during the completion of this work. C.G. acknowledges support from MPQ-ICFO, ICFOnest+ (FP7-PEOPLE-2013-COFUND), and cofunding by the European Union's Marie Skłodowska-Curie Individual Fellowships (IF-EF) programme under GA: 700140, as well as from the European Research Council (ERC AdG OSYRIS and CoG QITBOX), Axa Chair in Quantum Information Science, The John Templeton Foundation, Spanish MINECO (FOQUSFIS2013-46768 and Severo Ochoa Grant No. SEV-2015-0522), Fundació Privada Cellex, and Generalitat de Catalunya (Grant No. SGR 874 and 875). This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant Agreement No. 694925).

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