Entanglement of mid-spectrum eigenstates of chaotic many-body systems — reasons for deviation from random ensembles

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Eigenstates of local many-body interacting systems that are far from spectral edges are thought to be ergodic and close to being random states. This is consistent with the eigenstate thermalization hypothesis and volume-law scaling of entanglement. We point out that systematic departures from complete randomness are generically present in mid-spectrum eigenstates, and focus on the departure of the entanglement entropy from the randomstate prediction. We show that the departure is (partly) due to spatial correlations and due to orthogonality to the eigenstates at the spectral edge, which imposes structure on the mid-spectrum eigenstates.

I. INTRODUCTION

Ergodicity and equilibration in the quantum realm remain imperfectly understood, and the characterization of quantum ergodicity is now an active research front. One view is that quantum ergodicity corresponds to eigenstates of many-body systems being effectively random. This idea is closely connected to the eigenstate thermalization hypothesis (ETH) [1-7], and to ideas loosely known as (canonical) typicality [7-18]. For a non-integrable (chaotic) many-body Hamiltonian H, it is expected that a state $|\psi_R\rangle$ with independent Gaussian random coefficients should be a good model for infinite-temperature eigenstates, while eigenstates at energy corresponding to temperature $1/\beta$ should be well-described by $e^{-\frac{1}{2}\beta H} |\psi_R\rangle$ [17, 19– 22]. This expectation is mirrored by the behavior of the entanglement entropy (EE) in eigenstates of many-body systems with finite Hilbert spaces: At the spectral edges, EE is low ("area law") [23, 24], while in the infinite-temperature (midspectrum) regime, the eigenstates have EE close to the value expected for random states. As a result, for chaotic manybody systems, the scatter plot of EE versus eigenenergy takes the shape of an arch or rainbow, by now familiar from many numerical examples [25-37].

In this work, we consider the bipartite entanglement entropy of mid-spectrum eigenstates. For definiteness, we focus on spin-1/2 chains with L sites with all symmetries broken, so that the Hilbert space is $D = 2^L$, and consider the entanglement between two subsystems (A, B) of equal size. In this case, the random states have an average EE well-approximated by the Page formula [38, 39], $S_{Page} = \log D_A - \frac{1}{2}$, where $D_A = 2^{L/2}$ is the size of the reduced Hilbert space of the A subsystem. Although the mid-spectrum eigenstates are expected to be random, numerically calculated mid-spectrum entanglement in finite-size many-body systems - both in the existing literature [25, 40, 41] and in this work – systematically fall below the Page value. The deviation decreases more slowly with system size than the width of the state-to-state fluctuations of EEs, which means that the deviation is significant at *any* finite size. To the best of our knowledge, the origin of this subtle, systematic and seemingly universal effect has not been addressed so far. In this work, we present a study of this discrepancy, un-



FIG. 1. Schematic, summarizing main ideas. Lower rainbow shows block EE against eigenenergies. Upper rainbow is EE between "comb" partitions. Partitions are shown in the left and right insets, respectively. The difference between the top of the two rainbows is attributed to residual spatial correlation in mid-spectrum eigenstates. The difference between the Page value (dotted horizontal line) and the mid-spectrum comb entanglement is attributed to the "orthogonality blockade" effect — orthogonality to the special spectral edge states. 3D plots are cartoons of distributions of eigenstate intensities, using a 2D space to visualize the Hilbert space. The three cases correspond to low-entanglement states typical of spectral edges (middle), fully random or 'ergodic' states (right), and mid-spectrum states (left). The latter demonstrates a depletion of weight in parts of the Hilbert space where the spectral edges have large weight.

covering the ways in which mid-spectrum eigenstates deviate from random states.

We find that the *locality* of the Hamiltonian leads to *spatial correlations* persisting in mid-spectrum eigenstates of any finite system; we demonstrate this through the mutual information between sites. The mid-spectrum eigenstates thus differ in an important manner from random states. The presence of spatial correlations manifests itself strongly in the entanglement between spatially connected blocks (*block* bipartition) – a partitioning which is naturally sensitive to spatial correlations in eigenstates. We show that the departure of mid-spectrum entanglement from the Page value is smaller for *comb* partitions that are, of all bipartitions, the least sensitive to spatial variations of correlations. Nevertheless, even the comb entanglements depart from the Page value. We argue that the reason for the departure from Page value of the mid-spectrum eigenstates is their orthogonality to the eigenstates at spectral edges. Orthogonality forces the mid-spectrum eigenstates to live in an effectively lower-dimensional Hilbert space: part of the physical Hilbert space is blocked off. This Hilbert space blockade phenomenon manifests itself in the eigenstate coefficient distribution as an enhanced weight around zero [42–45]. The orthogonality blockade effect exists for any Hamiltonian, local or not. However, for local Hamiltonians, eigenstates at the spectral edges have area law entanglement and strong spatial correlations. The blockade effect then forces mid-spectrum states to have the observed spatial correlations. The departure from the Page value for comb partitions is thus due to a correlated Hilbert space blockade, such that certain types of configurations in the Hilbert space are blocked from appearing in the mid-spectrum eigenstates. This scenario is illustrated in Fig. 1 and elaborated in the rest of this paper.

II. MODEL

We focus on the spin- $\frac{1}{2}$ chain, with couplings between sites i, j having the XYZ form $h_{i,j}[\eta, \Delta] = (1 - \eta)S_i^x S_j^x + (1 + \eta)S_i^y S_j^y + \Delta S_i^z S_j^z$. The nearest-neighbor version of this model is integrable through the algebraic Bethe ansatz [46]. Since our focus is on non-integrable systems, we add next-nearest neighbor couplings $h_{j,j+2}$ and/or magnetic fields:

$$H = J_1 \sum_{j=1}^{L-1} h_{j,j+1}[\eta_1, \Delta_1] + J_2 \sum_{j=2}^{L-2} h_{j,j+2}[\eta_2, \Delta_2] + h_z \sum_{j=1}^{L} (1 - \frac{1}{2}\delta_{jL})S_j^z + h_x \sum_{j=1}^{L} (1 - \frac{1}{2}\delta_{j1})S_j^x.$$
 (1)

The h_x term breaks the parity of total- S^z . In addition, the J_2 , h_z and h_x terms are each tweaked at one edge of the chain so that reflection symmetry is broken. Unless otherwise specified, we present data for $J_\alpha = 1$, $\eta_\alpha = 0.5$, $\Delta_\alpha = 0.9$, $h_z = 0.8$, $h_x = 0.2$. For parameters that we used, the level spacing statistics of the model is consistent with that of the Gaussian orthogonal ensemble (GOE), indicating chaotic behavior.

III. ENTANGLEMENT FOR BLOCK PARTITIONS

In Fig. 2 we consider "block" bipartitioning, i.e., the A(B) bipartition is the left (right) half of the chain. The spectral edges and mid-spectrum states scale differently (~ L^0 vs ~ L^1), resulting in the rainbow/arch shape, Fig. 2(a-c). The largest EE values are close to the EE values of random states of the same Hilbert space size, whose average is here the Page value, $S_{\text{Page}} = \frac{L}{2} \ln 2 - \frac{1}{2}$, because we have chosen a spin- $\frac{1}{2}$ system with no symmetries. The EE being close to the Page value indicates that the mid-spectrum eigenstates are close to being "random" or "infinite-temperature". Accordingly, the width of the distribution of mid-spectrum EE values is expected to decrease as ~ $D^{-1/2}$, like eigenstates of GOE/GUE matrices



FIG. 2. EE for block bipartition. Parameters listed in text. (a-c) EE versus energy for different system sizes. Horizontal line: Page value. (d) Statistics of mid-spectrum eigenstates (D/16 states nearest to rainbow peak), for L = 8,10,12,14,16. The standard deviation has similar scaling ~ $D^{-1/2}$ to the GOE case. The departure from the Page value falls off much more slowly, possibly even saturating.

[47]. Fig. 2 (d) shows that the mid-spectrum EE widths are larger than corresponding GOE values, but are consistent with $\sim D^{-1/2}$ behavior.

The feature we focus on in this paper is the systematic departure from the Page value even in the middle of the spectrum (Fig. 2 (c) inset). Fig. 2 (d) shows how the departure of the mean mid-spectrum EE from the Page value scales with system size. There is some ambiguity in how to choose the "midspectrum" states. Fig. 2 (d) uses the 1/16th eigenstates closest to the top of the rainbow, but our observations are insensitive to the exact procedure [39]. The departure decreases with the system size *remarkably slowly*. In fact, the data does not rule out saturation, i.e., nonzero departure in the thermodynamic limit. The departure is certainly much larger than the width, which decreases much faster, ~ $D^{-1/2}$. Thus, at *any* system size, the Page value lies outside the distribution of EE values. In this sense, the departure is not "merely a finite size effect."

IV. SPATIAL CORRELATIONS AND COMB ENTANGLEMENT

To uncover the reason for the departure from random-matrix behavior, we first appeal to the best-known case of such departures, namely the spectral edges, for which the volume law of entanglement is violated [23, 24]. The origin of area law EE is the spatial locality of the Hamiltonian. This causes correlations to decay rapidly with distance, and ensures that the block entanglement receives its largest contribution from the boundary region. We ask whether some degree of locality, in this sense, also exists in the mid-spectrum eigenstates. We quantify correlations via the quantum mutual information

$$I(i, j) \equiv S_{[i]} + S_{[j]} - S_{[i \cup j]}$$
(2)

for pairs of spins *i* and *j*, as in [48, 49]. Fig. 3(a) shows I(i, j) against the distance |i - j|, for mid-spectrum eigenstates, low-energy eigenstates and random states. The distance dependence in mid-spectrum eigenstates is much less pronounced than in low-energy eigenstates, as expected. However, there exists an unmistakable dominance of small-distance cor-



FIG. 3. Spatial correlations and comb EE. (a) Mutual information vs. distance. Low-energy and mid-spectrum eigenstates of XYZ Hamiltonians, compared with eigenstates of full (GOE) and sparse random matrices. Statistics gathered from 32 eigenstates of each of 40 XYZ Hamiltonians, with parameters drawn from ranges shown. (b) EE for block and comb bipartitions. (c) Scaling of mid-spectrum comb EE (both types, filled/open symbols), similar to Fig. 2(d). The departure from the Page value falls much slower than the width.

relations. Thus, we identify distance-dependence as one reason for the departure of mid-spectrum EE from the Page value.

To 'correct' for this effect, we consider 'comb' bipartitions [50-54] of two types: 'comb1' partitions spins as *ABABAB*..., i.e., it is a sublattice partition, while 'comb2' partitions the spins as *AABBAABB*.... For comb2 partitioning, there is some ambiguity when *L* is not divisible by 4; we resolve this by setting the last two sites to be in partitions *A* and *B*. For example, for *L* = 10, the comb2 partitioning is *AABBAABBA*.

For such bipartitions, the EE should be insensitive to largescale distance-dependence of correlations, as two nearby points are as likely to be in different partitions as two faraway points. (The boundary and bulk of partitions are not spatially separated.) Fig. 3(b) shows that the mid-spectrum comb EE is indeed closer to the Page value than the block EE. There is little difference between comb1 and comb2, which supports the idea that this reduction of the departure is due to removal of the effect of distance-dependence. For comb bipartitioning, there is no notion of 'area law', so that the EE for spectral edges scale as ~ L instead of ~ L^0 . Nevertheless, the comb EE's at the spectral edges are significantly smaller than the mid-spectrum ones, despite having the same scaling. Thus the comb EE's are also arranged in an arch/rainbow shape [39].

Remarkably, even for comb partitions, the departure from the Page value remains much larger than the width of midspectrum EE distributions. As in the block case, the comb EE departure decreases far slower than the width, Fig. 3(c). (The available data would even be consistent with a *saturation* of the departure in the $L \rightarrow \infty$ limit, as opposed to a slow decrease.) Thus the departure is a visible effect at any finite size, also for partitions which (unlike block partitions) do not select for locality effects. We are thus forced to look for additional mechanisms – beyond 'locality' as discussed above – for the departure from the random-state behavior.

V. NON-EXPLANATIONS

Sparsity is not responsible — One possible source of the difference between random states and the eigenstates of local many-body Hamiltonians is that such Hamiltonians are generally sparse matrices in common basis choices. To examine the consequence of sparsity, in Fig. 3(a,b) we include results (mutual information, EE) for the eigenstates of matrices with sparsity close to the physical (XYZ) Hamiltonian, and nonzero elements drawn from a Gaussian distribution. We find only very slight differences from eigenstates of the usual (full) GOE ensemble — in Fig. 3(a) the mutual information values for the GOE case and the sparse random case are very slightly offset from each other (offset barely visible), while in Fig. 3(b) the EE values for the sparse random matrix have a distribution whose center is only very slightly lower than the page value.

Thus, sparsity is not a significant factor in the departure from the Page value.

Effect of finite measurement window — To obtain sufficient statistics for the average and width of mid-spectrum entanglements, we use the EE values within some energy window, $E_{\text{max}} - \Delta E/2 < E < E_{\text{max}} + \Delta E/2$, containing the energy E_{max} where the EE is maximal. Approximating the EE to be a smooth function of energy, S(E), the average EE within an energy window ΔE is obtained by Taylor expansion to be smaller than the maximum by the amount $S_{\text{Taylor}} = \frac{1}{24} |S''(E_{\text{max}})|(\Delta E)^2$. We are of course interested in the limit $\Delta E \rightarrow 0$, where this effect plays no role. To ensure that we have reached this limit, we have carefully checked that our extracted values of departure are independent of the ΔE value used numerically, and also that the Taylor correction term is orders of magnitude smaller than the departure, for the values of ΔE used numerically [39].

In addition, from Fig. 2(c) inset and from Fig. 3(b), it is visually obvious that the top of the rainbow itself deviates from the Page value, and that the effect is not due to averaging over a finite energy window.

VI. ORTHOGONALITY AND BLOCKADE

We now introduce a framework for discussing the deviation of mid-spectrum states from randomness (full ergodicity). Eigenstates at the spectral edges are well-known to be special – they have area-law instead of volume-law entanglement, and this is reflected in the local structure of correlations. These eigenstates may be seen as occupying a specific tiny part of the Hilbert space which promotes the special features. Because mid-spectrum eigenstates need to be orthogonal to these special states, they are forced to *exclude* that part of the Hilbert space. Thus mid-spectrum eigenstates are distributed in a large



FIG. 4. Orthogonality blockade, illustrated. (a) Eigenstate coefficient distribution, showing an excess of small values compared to Gaussian. Excess appears not to scale with system size. (b) Scatter-plot between eigenstate coefficients. Each point represents one real-space configuration. Coefficients of a mid-spectrum state against those of a low-energy (b1) and a high-energy (b2) state. Eigenstates (in brackets) labeled from 1 to $2^{10} = 1024$. (c) EE of states obtained by orthogonalizing a random state to *k* lowest-energy and *k* highest-energy eigenstates. k = 0 is a random state; $k = \frac{D}{2} - 1$ is essentially a mid-spectrum eigenstate. Inset: EE's averaged over 30 starting states. Dashed straight line is a visual guide.

fraction of, but not the complete, Hilbert space: part of the Hilbert space is blocked off.

This blockade phenomenon is illustrated in the cartoons of Fig. 1. If we use real-space configurations as the basis, then these cartoons over-simplify in showing the low-energy states as having exactly zero coefficients for most basis states. In reality, the low-energy eigenstates are not completely localized in configuration space — they have low but nonzero entanglement. In other words, their participation ratios [39] are much smaller than the random state value of D/3, but are still much larger than 1 [25].

Aspects of the blockade phenomenon are illustrated in Fig. 4. The coefficients of mid-spectrum eigenstates, in the basis of real-space configurations, are not entirely Gaussian (as would be the case for GOE eigenstates) but have excess weight at small values [42–45], Fig. 4(a). Some configurations are "overrepresented" in eigenstates at the spectral edges; hence by orthogonality they have to be under-represented in mid-spectrum eigenstates, leading to an excess of small values of coefficients. This effect is seen more explicitly when coefficient magnitudes of different eigenstates are plotted against each other – Fig. 4(b) shows that low/high-energy eigenstates have anomalously large weights in a few basis states, which have small weights in mid-spectrum eigenstates [39].

In Fig. 4(c) we show how orthogonality affects entanglement. Starting from a random state, we successively Gram-Schmidtorthogonalize against pairs of eigenstates at the outermost edges of the spectrum, i.e., first with the lowest and highest eigenstates, then with the second-lowest and second-highest eigenstates, and so on. The EE (both block and comb) of the resulting states, Fig. 4(c), start with zero departure and, after all but the mid-spectrum eigenstates have been orthogonalized away, end at roughly the values observed for the EE's of midspectrum eigenstates. The curve has fluctuations depending on the initial random state used, but the fluctuations decrease with increasing system size and the overall picture is valid for a variety of random states tried [39]. When averaged over various realizations of the starting random state, one obtains a relatively smooth curve, as shown in the inset.

For simplicity, we have above described the blockade as being due to only the eigenstates at the spectral edges. In truth, the mid-spectrum eigenstates are affected by orthogonality to all non-mid-spectrum eigenstates, not just those at the spectral edges. Intuitively, one might expect the spectral edges to have the strongest effect, as these eigenstates are the least generic or random-like. Comparing with the straight line in the inset to Fig. 4(c), we see that the slope of the curve is larger for small k, i.e., orthogonalizing against the spectral edges has a stronger effect than orthogonalizing against eigenstates which are intermediate between the spectral edges and the midspectrum region. This demonstrates that eigenstates closer to the spectral edges indeed have a stronger role in causing the mid-spectrum departure [39]. For simplicity, we sometimes loosely describe the blockade to be due to spectral edge states it should be understood that intermediate states also contribute to the phenomenon, albeit to a weaker degree.

Interestingly, the distribution of coefficients by itself does not predict the correct mid-spectrum EE. Using a random state with coefficients drawn from the observed mid-spectrum distribution, Fig. 4(a), we find the resulting EE to have a departure one order of magnitude smaller than that observed in the comb cases. Thus, a random state with an effective Hilbert space of reduced dimension $D_{\text{eff}} < D$ (as in [55]) is not sufficient to model the departure. The orthogonality causes very particular combinations of configurations to be missing from the midspectrum eigenstates; this "correlated blockade" is necessary for the observed departure [39].

VII. RAINBOW SHAPE IMPLIES DEPARTURE

The orthogonality mechanism has the following implication. If the EE versus eigenenergy plot is rainbow- or arch-shaped, then the correlations in spectral-edge eigenstates which cause those to have low entanglement will affect the mid-spectrum eigenstates by orthogonality, causing the mid-spectrum eigenstates to depart from Gaussian randomness. Thus, a rainbow shape is necessarily accompanied by a departure in the mid-spectrum states.

We can thus trace back the departure for comb EE to the fact that the EE plot is rainbow-shaped for comb bipartitioning. Unlike block partitioning, there is now no parametric argument ($\sim L^0 \text{ vs} \sim L^1$) for the rainbow shape, as the spectral edge EE now scales as $\sim L$ (the scaling of the boundary between partitions), the same as the mid-spectrum EE. A general argument for the rainbow shape is that, because the low-/high-energy states are more constrained (less like random states) compared to mid-spectrum eigenstates, the EE at spectral edges has to be farther from the Page value compared to mid-spectrum EE.



FIG. 5. (a) Power-law random banded matrix of size 2^{10} , treated as a 10-spin Hamiltonian. EE versus eigenvalues, for exponent α in the ergodic/delocalized (a1), weakly ergodic (a2) and localized (a3) regimes [39]. Case (a2) is analogous to the many-body situation. (b) Lines are block EE calculated from states $e^{-\frac{1}{2}\beta H} |\psi_R\rangle$, for different realizations of random $|\psi_R\rangle$. On average, these lie above actual eigenstate EE's at all temperatures/energies.

However, this is not obviously related to the spatial structure of correlations. In fact, in a model without spatial locality, where all eigenstates have volume-law scaling, the EE is found to also have a rainbow structure [40]. According to the picture presented above, orthogonality should then force a departure of the mid-spectrum EE; indeed this is observed [40].

Our picture is applicable also beyond the context of many-body physics. In power-law random banded matrices (PLRBMs) [49, 56–66] and ultrametric matrices [61– 64, 67, 68], there is a regime of parameters where the midspectrum eigenstates are "weakly ergodic" in the sense that, even though the scaling with matrix size matches the ergodic case, there is deviation from GOE/GUE ensembles at any finite size [44, 64, 66]. To connect to the present topic: by interpreting the indices of such matrices as spatial configurations (as discussed in, e.g., [39, 69, 70]), one can evaluate entanglements. For PLRBMs in the weakly ergodic regime, we have found a rainbow-shaped dependence of EE versus eigenenergy, with a mid-spectrum departure (Fig. 5(a) and [39]), just as in the many-body case. The spectral edges are likely power-lawlocalized [39], so that the blockade effect is more direct than in the many-body situation.

VIII. CONTEXT & CONSEQUENCES

The EE of non-extremal eigenstates is now the focus of considerable attention, both for chaotic systems [22, 25, 26, 40, 71–87] as in this work, and also for integrable systems [25, 40, 41, 70, 88–102]. The eigenstate EE plays a role in

connecting quantum properties to the thermodynamic entropy [9, 26, 72–74, 80, 92, 103]. Current theory suggests that the mid-spectrum states are effectively random. We have shown that a subleading deviation is present for any finite size, and have developed concepts (orthogonality blockade, residual spatial correlations) pertinent to understanding this deviation. We expect our results to be equally valid for systems with symmetries (for which the average random-state EE is not given by the Page formula), and that the presented concepts will have further applications, e.g., effects of orthogonality to the extremal eigenstates has been exploited in recent literature [66, 104–106]. An open question is whether the deviation *saturates* or vanishes in the large-size limit.

The idea that the state $e^{-\frac{1}{2}\beta H} |\psi_R\rangle$ (with $|\psi_R\rangle$ a random state) is a good model for finite-temperature eigenstates [17, 20, 22] has been fruitful for numerical computations of thermodynamic properties [107–118]. Our observation, that mid-spectrum (highest-EE or infinite-temperature) eigenstates show departures from random state properties, implies that the state $e^{-\frac{1}{2}\beta H} |\psi_R\rangle$ is an imperfect model for lower-entanglement (finite-temperature) eigenstates as well. In fact, one can attempt to reproduce the entanglement rainbow by plotting the EE of the state $e^{-\frac{1}{2}\beta H} |\psi_R\rangle$ against the corresponding energy. We find that this curve falls systematically above the EE scatterplot of actual eigenstates (Fig. 5(b) and [39]).

The departure is a signature of deviation from GOE/GUE behavior at all finite sizes. Signatures of this deviation also appear in eigenstate coefficient distributions (Fig. 4(a); also [42–45]). Mid-spectrum eigenstates have the same scaling behavior as GOE/GUE, but approach the thermodynamic limit differently, as also seen in multifractality analysis [44]. This behavior could justifiably be called "weakly ergodic", although the phrase does not yet have a widely accepted definition [44, 64, 66, 104, 119, 120]. In Ref. [120], weak ergodicity is associated with breaking of "basis rotation invariance." Our finding, that mid-spectrum eigenstates have different block EE and comb EE, is another type of non-invariance under basis rotation.

Note added in Proof: After this paper was accepted, we became aware of Ref. [121], which quantitatively accounts for part of the departure for block partitions, in the case where the Hamiltonian is local.

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