

Two-Component Structure in the Entanglement Spectrum of Highly Excited States

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(Received 30 July 2015; published 23 December 2015)

We study the entanglement spectrum of highly excited eigenstates of two known models that exhibit a many-body localization transition, namely the one-dimensional random-field Heisenberg model and the quantum random energy model. Our results indicate that the entanglement spectrum shows a “two-component” structure: a universal part that is associated with random matrix theory, and a nonuniversal part that is model dependent. The nonuniversal part manifests the deviation of the highly excited eigenstate from a true random state even in the thermalized phase where the eigenstate thermalization hypothesis holds. The fraction of the spectrum containing the universal part decreases as one approaches the critical point and vanishes in the localized phase in the thermodynamic limit. We use the universal part fraction to construct an order parameter for measuring the degree of randomness of a generic highly excited state, which is also a promising candidate for studying the many-body localization transition. Two toy models based on Rokhsar-Kivelson type wave functions are constructed and their entanglement spectra are shown to exhibit the same structure.

DOI: [10.1103/PhysRevLett.115.267206](https://doi.org/10.1103/PhysRevLett.115.267206)

PACS numbers: 75.10.Pq, 03.65.Ud, 05.30.Rt, 72.15.Rn

Introduction.—Quantum entanglement, a topic of much importance in quantum information theory, has also gained relevance in quantum many-body physics in the past few years [1,2]. In particular, the entanglement entropy provides a wealth of information about physical states, including novel ways to classify states of matter that do not have a local order parameter [3]. However, it has been realized only recently in various physical contexts that the entanglement entropy is not enough to fully characterize a generic quantum state. For example, the quantum complexity corresponding to the geometric structure of black holes cannot be fully encoded just by the entanglement entropy [4]. One natural step beyond the amount of entanglement is the specific pattern of entanglement, i.e., the entanglement spectrum. A recent result that motivates this direction is the relationship between irreversibility and entanglement spectrum statistics in quantum circuits [5,6]. It was shown that irreversible states display Wigner-Dyson statistics in the level spacing of entanglement eigenvalues, while reversible states show a deviation from Wigner-Dyson distributed entanglement levels and can be efficiently disentangled.

Are there universal features in the entanglement spectrum of a generic eigenstate of a quantum Hamiltonian? Highly excited eigenstates of a generic quantum Hamiltonian are believed to satisfy the “eigenstate thermalization hypothesis” (ETH) [7–9], which states that the expectation value $\langle \psi_\alpha | \hat{O} | \psi_\alpha \rangle$ of a few-body observable \hat{O} in an energy eigenstate $|\psi_\alpha\rangle$ of the Hamiltonian with energy E_α equals the microcanonical average at the mean energy E_α . So one could as well ask the following question: What

is the structure of the entanglement spectrum of highly excited eigenstates of a thermalized system? Here we find a quandary. Completely random states are generically not physical, namely, they cannot be the eigenstates of Hamiltonians with local interactions. For the ETH to be a physical scenario for thermalization, highly excited eigenstates of physical local Hamiltonians cannot always be completely random, yet they have to contain enough entropy. Deviations from a completely random state can be quantified by the entanglement entropy, more precisely by the amount that it deviates from the maximal entropy in the subsystem, derived by Page, which we will refer to as the Page entropy hereafter [10]. But are there features that cannot be captured by the entanglement entropy alone? Can one identify remnants of randomness in the full entanglement spectrum? What about in states that violate the ETH?

In this Letter, we address the above questions using as a case study the problem of many-body localization (MBL) [11–15]. We study two known models that were shown to exhibit a MBL transition, namely, the Heisenberg spin model with random fields, and the quantum random energy model (QREM) [16–18]. In the delocalized phase, high-energy eigenstates are thermalized according to the ETH. The deviation from completely random states manifests itself in a “two-component” structure in the entanglement spectrum: a universal part that corresponds to random matrix theory [19], and a nonuniversal part that is model dependent. We show that the universal part fraction decreases as one approaches the transition point and vanishes in the localized phase in the thermodynamic limit.

We therefore propose an order parameter that is able to measure the degree of randomness of a generic highly excited state and capture the many-body localization-delocalization transition based on the entanglement spectrum, and show that it gives predictions consistent with previous results. We further construct two toy models in terms of Rokhsar-Kivelson- (RK-)type wave functions [20,21] and the same structure in the entanglement spectra is observed.

Heisenberg spin chain.—A well-studied model that shows a MBL transition is the isotropic Heisenberg spin-1/2 chain with random fields along a fixed direction

$$\mathcal{H} = \sum_{i=1}^L (h_i S_i^z + J \vec{S}_i \cdot \vec{S}_{i+1} + \Gamma S_i^x), \quad (1)$$

where the random fields h_i are independent random variables at each site, drawn from a uniform distribution in the interval $[-h, h]$. Γ is a uniform transverse field along the x direction, which breaks total S_z conservation. We assume periodic boundary condition and set the coupling $J = 1$ and $\Gamma = 0.1$. In the absence of the transverse field Γ , previous work located the critical point at $h = h_c \approx 3.5$ in the $S_z = 0$ sector [13,22,23]. We consider two different regimes by varying the disorder strength parameter h : (i) within the thermalized phase ($h < h_c$), and (ii) in the localized phase ($h > h_c$). In each regime, we focus on eigenstates of the Hamiltonian (1) at the middle of the spectrum, namely, on highly excited states.

We consider a bipartition of the system into subsystems A and B of equal size ($L/2$ sites each). For a generic

eigenstate $|\psi\rangle = \sum_{\sigma} \psi(\sigma) |\sigma\rangle$, where $\sigma \equiv \sigma_1 \sigma_2 \cdots \sigma_L$ labels the 2^L possible spin configurations of the system, we cast the wave function as $\psi(\sigma) \equiv \psi(\sigma_A \sigma_B)$, where $\sigma_A \equiv \sigma_1 \cdots \sigma_{L/2}$ and $\sigma_B \equiv \sigma_{L/2+1} \cdots \sigma_L$. The entanglement spectrum is obtained from the eigenvalues of the reduced density matrices $\rho_A = \text{tr}_B |\psi\rangle\langle\psi|$ and $\rho_B = \text{tr}_A |\psi\rangle\langle\psi|$: $\{p_k = \lambda_k^2\}$, $k = 1, \dots, 2^{L/2}$. In this work, we are primarily concerned with the density of states and level statistics of the $\{\lambda_k\}$ for highly excited eigenstates for different strengths of disorder. For each value of h analyzed, the spectra were averaged over 10 realizations of disorder for $L = 16$, and 100 realizations for $L = 14$. For each spectrum, the eigenstate with energy closest to zero was obtained by a Lanczos projection [24]. This eigenstate corresponds to a highly excited state.

Thermalized phase.—We start by considering the weakly disordered case $h \ll h_c$. Only a small amount of disorder is necessary to break the integrability of the clean Hamiltonian. However, conservation of the total S_z also plays a crucial role in making eigenstates completely random. A small transverse field Γ is applied to break this conservation without substantially altering the many-body localization transition. In this regime, we find that the entanglement spectrum of the highly excited state with eigenenergy near zero is close to that of a completely random quantum state, as shown in Fig. 1(a) for systems of size $L = 16$ and $h = 0.5$. The entanglement spectrum follows closely a Marchenko-Pastur distribution (with proper normalization), which describes the asymptotic average density of eigenvalues of a Wishart matrix [25,26]. (The expression for the entanglement spectral

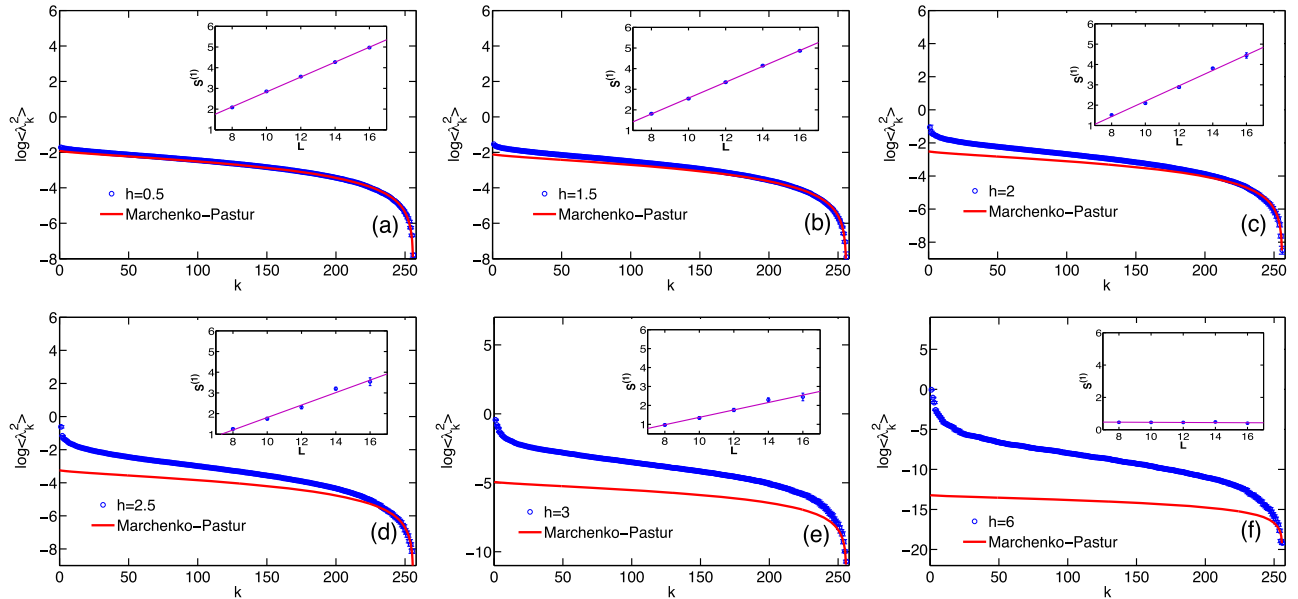


FIG. 1 (color online). Average entanglement spectrum of highly excited eigenstates for a system of size $L = 16$, averaged over ten realizations of disorder (plotted in logarithmic scale). Panels (a)–(f) show the spectrum for $h = 0.5, 1.5, 2, 2.5, 3,$ and 6 , respectively. The solid lines correspond to the spectrum of a completely random state (derived from a Marchenko-Pastur distribution), and is shown for reference. Insets: scaling of the average entanglement entropy $S^{(1)}$ with system size.

density for the random state is presented in the Supplemental Material [27]). One can also check that, in this regime, the von Neumann entanglement entropy $S^{(1)} = -\sum_k p_k \ln p_k$ is in good agreement with the Page entropy for random states: $S_{m,n} = \sum_{k=n+1}^{mn} (1/k) - (m - 1/2n) \approx \ln(m) - (m/2n)$, where m and n are the Hilbert space dimensions of subsystem A and B , respectively [10]. For example, our computed average entropy for 16 sites is $\langle S^{(1)} \rangle = 4.9719 \pm 0.0015$, while the corresponding Page entropy is $S_{\text{Page}} = 5.0452$.

As the disorder strength is increased, but still $h < h_c$, the system remains in the thermalized phase where it is supposed to obey the ETH and yield volume-law scaling of the entanglement entropy with system sizes [30], which is verified in the insets of Figs. 1(a) to 1(e). However, in spite of the volume-law scaling of the entanglement entropy and the thermalization of eigenstates, the entanglement entropy is much lower than the Page entropy. This indicates that the pattern of entanglement must have changed, which is manifest in the spectra shown in Figs. 1(b) to 1(e). The entanglement spectrum shows a striking “two-component” structure: (i) a universal tail in agreement with random matrix theory, and (ii) a nonuniversal part. The nonuniversal part dominates the weights in the spectrum (large λ_k values), resulting in low entanglement entropy, as it decays much faster than the universal part. Therefore, we find that although thermalized states are not necessarily random states, they partially retain a component that is reminiscent of a random state: the entanglement spectrum follows the Marchenko-Pastur level density distribution. In addition, the universal part of the entanglement spectrum follows a Wigner-Dyson distribution of level spacings (see the Supplemental Material [27]).

Localized phase.—In this regime, the entanglement entropy exhibits an area-law scaling with the system size [see the inset of Fig. 1(f)], which in one spatial dimension implies a constant entropy and, at most, weakly logarithmic corrections, in accordance with Ref. [31].

The entanglement spectrum in the localized regime, depicted in Fig. 1(f) for $h = 6$, shows a different scenario from that in the thermalized phase: the universal part of the spectrum disappears completely, leaving only the nonuniversal part characterized by its fast decay rate.

QREM.—The QREM describes L spins in a transverse field Γ with the following Hamiltonian:

$$\mathcal{H} = E(\{\sigma^z\}) + \Gamma \sum_{i=1}^L \sigma_i^x, \quad (2)$$

where $E(\{\sigma^z\})$ is the classical REM term that takes independent values from a Gaussian distribution of zero mean and variance $L/2$ [32]. This model was first studied in the context of a mean-field spin glass, and was shown to exhibit a first-order quantum phase transition as a function of Γ [16]. More recently, it was further demonstrated to

have a MBL transition when viewed as a closed quantum system [17]. Numerical and analytical arguments show that the transition happens at an energy density $|\epsilon| = \Gamma$ in the microcanonical ensemble. Since there is no support for the many-body localized phase at energy density $\epsilon = 0$, we examine the eigenstates with energy density closest to $\epsilon = 0.5$ instead, and study the entanglement spectrum as Γ is tuned. The two-component structure and its evolution as a function of Γ similar to Fig. 1 are again observed (see the Supplemental Material [27]).

An order parameter.—The above picture unveils a new aspect of the MBL transition. The two parts of the entanglement spectrum of a highly excited state clearly evolve as the disorder strength h is increased, namely, the universal part shrinks and the nonuniversal part grows. This fact suggests that one could use the fraction of each component as an order parameter.

Figures 1(a) to 1(e) indicate an h dependent value k_h that separates the nonuniversal ($k \leq k_h$) from the universal ($k > k_h$) parts of the rank-ordered entanglement levels (see the Supplemental Material [27] for the protocol for determining k_h). One can thus define the partial Rényi entropies

$$S_{\leq}^{(q)} = \frac{1}{1-q} \ln \sum_{k \leq k_h} p_k^q \quad (3)$$

with $q \geq 0$. Because the universal part of the spectrum is where the eigenvalues with low entanglement reside, this part of the spectrum is obscured by any measure that relies on the eigenvalues as weights. A good measure of the fraction of the two components that does not depend on these weights is given by the $q = 0$ Rényi entropy, which simply measures the ranks: $S_{\leq}^{(0)} = \ln k_h$. Therefore, an order parameter that measures the fraction of the universal component is

$$\mathcal{O}_{\text{MBL}} = 1 - \frac{S_{\leq}^{(0)}}{S^{(0)}} = 1 - \frac{\log_2 k_h}{L/2}. \quad (4)$$

Figure 2 shows the order parameter as defined above for the Heisenberg spin model and the QREM, respectively. For the QREM, all curves at different system sizes cross at $\Gamma_c \approx 0.5$, in excellent agreement with Ref. [17]. We have also looked at energy density $\epsilon = 0.3$, and the curves cross at $\Gamma_c \approx 0.25$, giving the same numerical prediction as in Refs. [17] and [18] (plot shown in the Supplemental Material [27]). For the random-field Heisenberg model, however, the fact that the transition happens at the point where the order parameter is nearly zero makes it harder to accurately locate the critical point using our order parameter. We see from Fig. 2 that the curves cross at $h_c \approx 3.3$, which is also consistent with previous studies. This indicates that, by considering the full entanglement

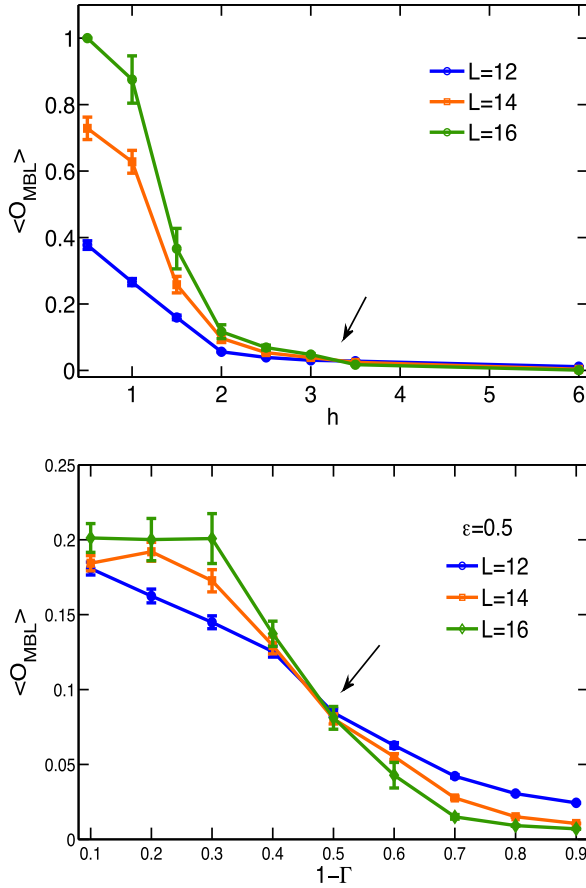


FIG. 2 (color online). The order parameter defined as the fraction of the universal component in the full entanglement spectrum for the Heisenberg spin model (upper panel) and the QREM (lower panel).

spectrum at high energies, our order parameter reveals a novel property that is promising for studying the MBL transition.

We remark that, although the MBL transition can also be captured by the scaling property of the entanglement entropy, our order parameter seems to be applicable even for models with nonlocal interactions, which could obscure the connection between the volume-to-area law transition of the entropy and the MBL transition.

Toy models.—We construct two RK-type model wave functions that are shown to have (i) the two-component structure in their entanglement spectra, and (ii) a phase transition as a function of the tuning parameter. The wave functions take the following form:

$$|\Psi\rangle = \frac{1}{\sqrt{\mathcal{Z}}} \sum_{\sigma} s_{\sigma} e^{-(\beta/2)E(\sigma)} |\sigma\rangle, \quad (5)$$

where $E(\sigma)$ is the energy for the classical configuration σ and \mathcal{Z} is the corresponding partition function of the classical statistical system [21]. s_{σ} is a random sign for each configuration, such that the wave function represents a

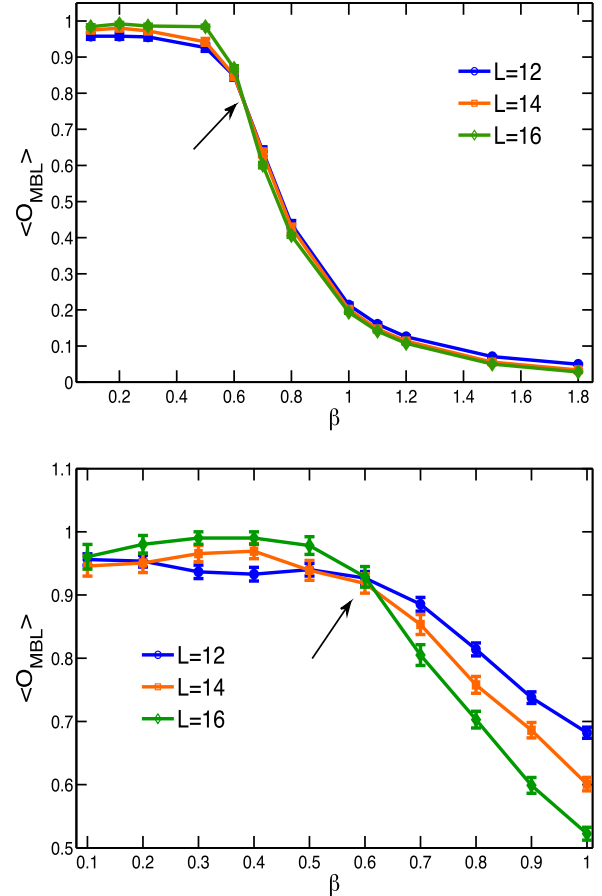


FIG. 3 (color online). The order parameter for the random-sign RK-type wave functions. Upper panel: $E(\sigma) = E_{\text{REM}}(\sigma)$. Lower panel: $E(\sigma) = -(J/L)\sum_{i<j}\sigma_i^z\sigma_j^z$ with $J = 1$.

highly excited state. We consider the following two cases: (i) $E(\sigma) = E_{\text{REM}}(\sigma)$, and (ii) $E(\sigma) = -(J/L)\sum_{i<j}\sigma_i^z\sigma_j^z$. In the first case, the energy is taken to be that of the REM, while in the second case the energy is that of an infinite-range uniform ferromagnetic interaction.

In the small β regime, the above RK-type wave functions are close to completely random states; upon increasing β , the wave functions are pushed towards product states and start to deviate from completely random states. Therefore, the tuning parameter β here plays the role of the “disorder strength.” Indeed, we find the same two-component structure in the entanglement spectrum (see the Supplemental Material [27]), and the order parameter is shown in Fig. 3. The REM case was recently studied by Chen *et al.* where the MBL transition was obtained numerically using other measures [33]. Here, we clearly see that, in both cases, the curves cross at some critical β , indicating the existence of a similar phase transition.

Summary and discussion.—The details of the structure of the entanglement spectrum, especially the universal part at the tails of the spectrum, have long been overlooked. The main focus has been primarily on the dominating

nonuniversal component, and the universal tail has thus far been discarded. For example, in the density matrix renormalization group [34] and tensor network methods [35], the density matrix is truncated to avoid uncontrolled growth of its dimensions. While this procedure is certainly justified when the purpose is to obtain ground state properties, it discards important information about the behavior of the system at higher energy states. In this Letter we showed that the full entanglement spectrum, directly computable from the wave function, provides information that is often invisible in the entanglement entropy alone.

On the other hand, much has been known about random quantum states, e.g., the Page entropy and volume-law scaling entropy. Nevertheless, the Page entropy is often an overestimate of the actual entanglement entropy computed from generic quantum states. Therefore, a natural question that arises is as follows: How random does a given quantum state look? In this Letter, we show that a generic quantum state that satisfies the ETH does not necessarily mean a completely random state. We present an order parameter to quantify the degree of randomness by using information about the full entanglement spectrum. In the context of MBL, our order parameter is able to locate the critical point, consistent with previous results. Our work may provide a novel way of studying MBL, and may shed new light on the understanding of many-body systems at the level of wave functions.

Z.-C. Y. is indebted to Bernardo Zubillaga, Alexandre Day, Shenxiu Liu, and Yi-Zhuang You for generous help and useful discussions. We thank Christopher Laumann for useful comments. This work was supported in part by DOE Grant No. DEF-06ER46316 (C. C.), by NSF Grant No. CCF 1117241 (E. R. M.), by National Basic Research Program of China Grants No. 2011CBA00300 and No. 2011CBA00301, and by National Natural Science Foundation of China Grant No. 61361136003 (A. H.).

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