Early Breakdown of Area-Law Entanglement at the Many-Body Delocalization Transition

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We introduce the numerical linked cluster expansion as a controlled numerical tool for the study of the many-body localization transition in a disordered system with continuous nonperturbative disorder. Our approach works directly in the thermodynamic limit, in any spatial dimension, and does not rely on any finite size scaling procedure. We study the onset of many-body delocalization through the breakdown of area-law entanglement in a generic many-body eigenstate. By looking for initial signs of an instability of the localized phase, we obtain a value for the critical disorder, which we believe should be a lower bound for the true value, that is higher than current best estimates from finite size studies. This implies that most current methods tend to overestimate the extent of the localized phase due to finite size effects making the localized phase appear stable at small length scales. We also study the mobility edge in these systems as a function of energy density, and we find that our conclusion is the same at all examined energies.

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Introduction.—The eigenstate thermalization hypothesis (ETH) is a powerful statement relating observables of the high energy eigenstates of a quantum many-body system with their thermal expectation values [1,2]. However, this principle can be violated in certain systems with strong enough disorder, where even the high energy eigenstates possess only local entanglement [3,4]. Anderson localization is a one-body example of this. An area of key interest is how far this localization persists in a many-body state in the presence of interactions [5]. At what point are interactions strong enough that the localization is destroyed and the system obeys ETH? This is the problem of the many-body localization (MBL) transition, which is a topic of active research both theoretically and experimentally [6–31].

The surge of interest in many-body localized systems has motivated many numerical studies. Most studies have focused on exact diagonalization or Lanczos methods which are able to address both sides of the transition in small systems [32–45]. However, since much about this phase transition is still not well understood, extension of finite size results to the thermodynamic limit can prove difficult. We would like to examine this phase transition using expansion methods, which provide an alternate way of addressing the thermodynamic limit. While standard perturbative series expansions are very powerful [46–48], they suffer from small energy denominators in models with continuous nonperturbative disorder. Thus, we turn to the numerical linked cluster (NLC) expansion [49–51], which does not suffer from this problem of small energy denominators.

In this Letter, we provide evidence that for a prototypical model of MBL, approaching the critical disorder from the localized side, the localized phase actually becomes unstable only at increasingly long length scales inaccessible to most numerical techniques. This implies that finite size numerical studies on the MBL transition tend to overestimate the extent of the localized phase.

Model.—The system we study explicitly is the spin-1/2 Heisenberg Hamiltonian with random fields along the z direction,

$$\mathcal{H} = \sum_i h_i S_i^z + \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

on the 1D chain, where the sum $\langle i, j\rangle$ is over adjacent pairs. The random field is picked from a uniform distribution $h_i \in [-h, h]$. This is one of the simplest models to study many-body localization on, and it has been studied numerically in great detail [32–35,52,53]. At low h, the system is in a thermalizing phase obeying the ETH while at high h, the system is in the localized (MBL) phase.

To identify these different phases, we focus on the entanglement properties of the eigenstates. The typical measure for entanglement in a pure state bipartitioned into two parts A and B is the von Neumann entropy, defined for some state $|\Psi\rangle$ as

$$s(|\Psi\rangle) = -\mathrm{Tr}(\rho_A \ln \rho_A), \tag{2}$$

where $\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$ is the reduced density matrix, obtained by tracing over all external degrees of freedom from the density matrix.

A typical eigenstate in an ETH obeying system will exhibit thermal volume-law entanglement. The entanglement entropy will approach the classical thermal entropy (required by ETH) and scale with the volume of the regions A and B. In the localized phase, the eigenstates will instead obey an area law, scaling with the area between A and B. This can be understood by regarding them as simultaneous eigenstates of many local operators [3]: only due to mixing contained in operators near the boundary will one get

contributions to the entanglement, which therefore grows with the area of the bipartitioning.

Numerical linked cluster expansions.—The NLC is similar to perturbative series expansions in that interactions within clusters of increasing size must be considered, but rather than perturbatively treating each interaction within a cluster, we solve them numerically, typically by exact diagonalization. Our treatment of disorder in the NLC is different from usual [51,54], allowing us to deal with continuous nonperturbative disorder. The procedure is outlined briefly here.

Let N be the order to which we wish to do the calculation. The order of the calculation is defined as the number of spins in the largest cluster considered. We identify a finite size region of the infinite system to work with. For the chain, this is simply a $2(N-1)$ length chain, with a bipartitioning cut in the middle. Each of the sites i is assigned a field h_i, which is held fixed until the calculation is complete. This choice of system size is used so that the results remain correct for the infinite system, to the desired order, as explained later.

We define a cluster c to be a set of sites. A Hamiltonian $\mathcal{H}_c$ can be obtained considering only the spins in c and can be diagonalized numerically to obtain the eigenstates $\{|\alpha^c\rangle\}$ with eigenvalues $\{\epsilon_\alpha^c\}$ labeled by α. Our quantity of interest, the eigenstate averaged entanglement entropy, can then be calculated as

$$S(c) = \sum_\alpha \frac{e^{-\beta\epsilon_\alpha^c}}{\mathcal{Z}} s(|\alpha^c\rangle), \tag{3}$$

where $\mathcal{Z} = \sum_\alpha e^{-\beta\epsilon_\alpha^c}$ is the normalization factor and $\beta = 1/T$ is the inverse temperature.

The entropy for the infinite lattice $\mathcal{L}$ can be expressed as a sum over the weight $\tilde{S}(c)$ of all clusters c that can be embedded in the lattice: $S(\mathcal{L}) = \sum_c \tilde{S}(c)$. The weight of a cluster is then defined recursively by the principle of inclusion and exclusion [49]:

$$\tilde{S}(c) = S(c) - \sum_{c' \subset c} \tilde{S}(c'). \tag{4}$$

One can show that only connected clusters which cross the boundary can have a nonzero weight. First, if a cluster does not cross the boundary, there can obviously be no entanglement in it or its subclusters, so the weight is trivially zero. Second, proving that only connected clusters can contribute simply amounts to proving that S obeys the linked cluster property, that is, for a cluster with two disconnected components c_1 and c_2, $S(c_1 \cup c_2) = S(c_1) + S(c_2)$. This follows from the fact that $\mathcal{H}_{c_1 \cup c_2} = \mathcal{H}_{c_1} \oplus \mathcal{H}_{c_2}$. Thus, we must simply consider connected clusters of up to size N that have sites on both sides of the partition. Our finite size representation was chosen to contain all of the necessary clusters of the infinite system up to order N. The count for the clusters crossing the boundary scales with the area, thus guaranteeing an area law as long as the NLC converges.

Using this, we can obtain a series a_n whose sum gives the total eigenstate averaged entanglement entropy per unit area S_{area},

$$S_{\text{area}} = \frac{1}{L_{\text{cut}}} \sum_{n=0}^{N} a_n; \qquad a_n = \sum_{c,|c|=n} \tilde{S}(c), \tag{5}$$

where L_{cut} is simply 1 for the chain. Finally, the entire calculation must be repeated for different realizations of $\{h_i\}$ to obtain a disorder averaged value for a_n [55].

The NLC scheme used here is slightly different from what has typically been used for random systems in the past, where different embeddings of the same graph are treated identically and one does not need a consistent finite system [54,56,57]. The more standard scheme has been applied to study MBL systems with discrete disorder [51], which allows one to perform disorder averaging before subgraph subtraction. When there is continuous disorder, partial disorder averaging over a finite number of realizations means that the linked cluster property is only approximate, and thus large errors will build up at high orders. In our approach, the linked cluster property is guaranteed and one is free to average over many realizations of the system. This is a key aspect of our calculation which allows us to treat disordered systems with continuous nonperturbative randomness.

Does it converge?—We first examine $T = \infty$. If entanglement satisfies a thermal volume law, interpreting n as a proxy length scale [50], we expect a_n to eventually saturate to the volume-law constant $\ln(2)/2$ for high enough n [58]. We should note that our model [Eq. (1)] does not possess a strongly thermalizing regime, due to the integrability at $h = 0$, and therefore we do not yet see this saturation to the thermal value within our range of n's [59]. In the localized phase, the additional entanglement due to the addition of one site far away from the cut should become exponentially small with distance, so we expect a_n to decay exponentially to 0 once n is larger than some localization length ξ. We define the MBL phase in our study to be one in which the sum of a_n converges exponentially.

Figure 1 shows a_n for a range of h values. To estimate convergence or divergence, a linear extrapolation to $1/n = 0$ can be performed. If the extrapolation predicts $a_\infty \geq 0$, we argue that this corresponds to a breakdown of area law. Although we expect a_n to eventually go to 0 exponentially in the localized phase, this would only happen when our cluster sizes are much greater than the localization length scale. This can be more clearly shown by examining the ratio of terms, which we will discuss next. Note that the case of an area law with logarithmic corrections would correspond to one where a_n heads linearly to 0, which we consider in this analysis to be the boundary between convergence and divergence.

Let us define the ratio of the (disorder averaged) series terms $r_n = a_n/a_{n-1}$. In the MBL phase, we can say more about the overall trend of r_n. Again interpreting n as a proxy length scale, for large n, we expect a_n to decrease exponentially with potentially power-law prefactors. The leading contributions at $n \gg \xi$ should be of the form $a_n = Cn^{-k}\exp(-n/\xi)$, where k is some positive number, ξ is the localization length, and C is some arbitrary constant [3]. Therefore, in the large n limit, discarding terms smaller than $1/n$, we expect

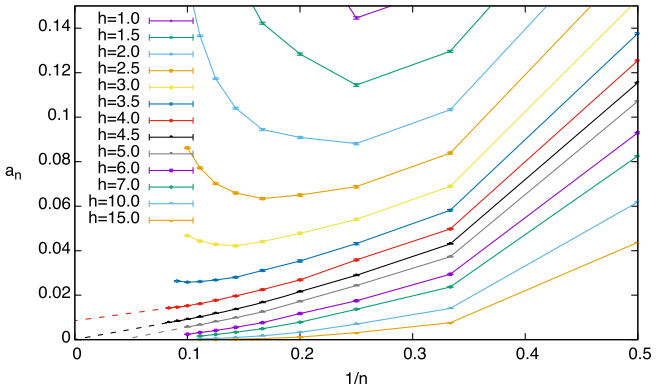

FIG. 1 (color online). The nth order area-law contribution a_n [Eq. (5)] at $T = \infty$. Near h_c, data has been averaged over more than 3×10^5 disorder realizations of the chain, and error bars show the standard error of the mean. The dashed lines are a demonstration of the linear extrapolation to a_∞ by fitting the last four terms in the series.

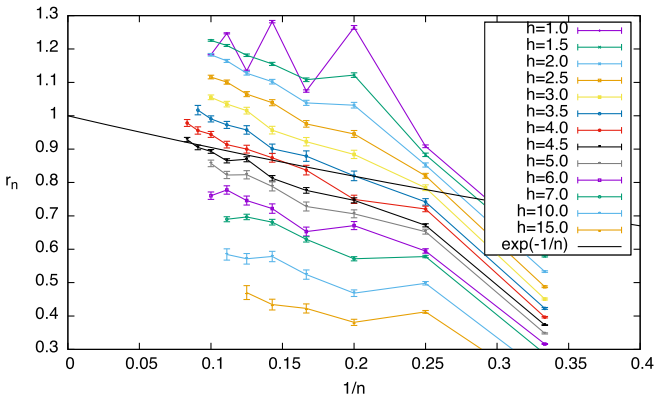

FIG. 2 (color online). Plot of the ratios $r_n = a_n/a_{n-1}$ versus $1/n$. Also shown is the line $\exp(-1/n)$, above which we argue that the expansion cannot converge exponentially.

$$r_n = a_n/a_{n-1} = (1 - k/n)\exp(-1/\xi). \tag{6}$$

Therefore, plotting r_n versus $1/n$, r_n should approach $r_\infty = \exp(-1/\xi)$ from below, with a slope of $-k$. However, near the transition, ξ can become very large and we do not actually see this behavior within our range of attainable n's. We can, however, predict whether this kind of exponential convergence is possible given the behavior of the series at a finite n.

Figure 2 shows the behavior of r_n for our range of h's and n's. The trend seems to be for r_n to increase steadily with n (although eventually r_n must approach 1 in the delocalized phase). If the system is in the MBL phase and the series is to converge exponentially, we expect that at some $n \gg \xi$, a_n will begin decreasing exponentially and r_n will begin heading towards r_∞ with slope $-k$. Barring bizarre behavior such as r_n increasing to some high value and then suddenly decreasing before finally increasing again towards r_∞, this places a restriction on what r_n can be when a_n begins its exponential decay. Because the slope of the approach is negative or 0, $r_n \leq r_\infty$. But also, $n \gg \xi$, which means that this decay can only begin occurring when

$$r_n \leq r_\infty = \exp(-1/\xi) < \exp(-1/n). \tag{7}$$

Therefore, once r_n has increased above $\exp(-1/n)$, a_n cannot converge exponentially. This is not a rigorous claim, but it should be valid as long as a_n behaves in a regular manner. This clearly shows (in Fig. 2) that the series for $h = 4.0$ cannot converge exponentially and thus is not in the MBL phase. However, the series for $h > 4.5$ are still within this region and thus may diverge or converge. Hence, our result should serve as a lower bound, with our best estimate being at $h_c = 4.5 \pm 0.1$. Going to higher order in the NLC can further refine this value.

Discussion.—A way of viewing our result [60] is that we are seeing an instability to thermalization of an almost-localized regime [61]. That is (in Fig. 1), initially a_n acts quite localized in that it is much smaller than the thermal value and is getting smaller as n is increased, but it may start increasing at higher n's, signaling the onset of thermalization. This onset of thermalization moves to a higher n as h is increased, but it goes beyond our range of accessible n after $h = 3.5$. However, by looking in a sensitive way for initial signs of an instability, we are able to place a lower bound for h_c at 4.5 ± 0.1.

To understand how our analysis is more sensitive to this transition than other methods, let us focus on the entanglement per unit volume S_{vol}. S_{vol} decreasing with system size is often associated with area-law entanglement, and therefore localization [33]. In our study, S_{vol} for a system of size N would correspond to the quantity $S_{\text{vol}} = (1/N)\sum_{n=0}^{N} a_n$. So even if a_n had already turned up and was increasing (clearly thermalizing), S_{vol} would not begin increasing until a_n had increased above the mean of all of the previous terms in the series. Our analysis predicts this upturn, which itself would precede estimates from finite size systems using S_{vol}.

Other methods, which are more focused on seeing the full onset of thermalization, do not observe the transition near our bound [32–35]. Results from Lanczos on systems of up to 22 sites with finite size scaling show evidence for a transition at $h_c \approx 3.7$ [33]. However, the scaling exponent $\xi \sim (h - h_c)^{-\nu}$ obtained from finite size scaling strongly violates the Harris-Chayes bound in one dimension [62,63], evidence that perhaps they are still far from the true critical point. This implies that finite size effects are significant, even in the systems accessible to Lanczos, and some corrections to the finite size scaling are needed. These effects cause an overestimate of the stability of the MBL phase, which actually becomes unstable to thermalization earlier only at much longer length scales. Note that an interesting alternate possibility is the existence of an intermediate phase between the ETH and the MBL phase, with neither thermal nor area-law entanglement [64–66], which we do not pursue further.

This onset of thermalization at high order is what one would expect from a long length scale delocalization mechanism. In studies of this transition using a renormalization group approach, one also finds that the transition is driven by rare metallic inclusions [67,68]. Near the transition, these are rare enough that small systems look localized but actually become thermalizing at long length scales.

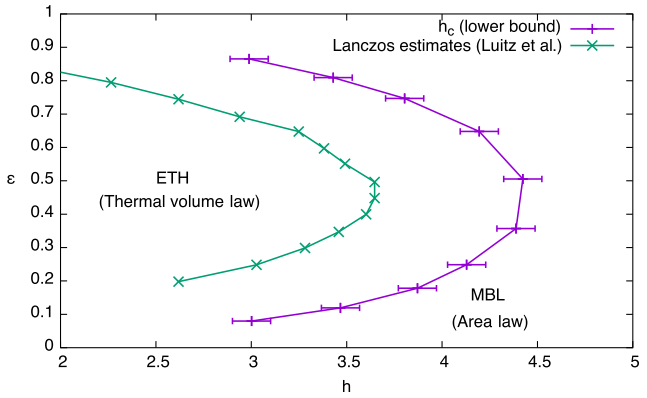

FIG. 3 (color online). The phase diagram with (scaled) energy and disorder on the axes, identified by interpolation of the intercept method (Fig. 1) up to order 10. Error bars represent confidence in our interpolation. Also shown is the h_c obtained by finite size scaling of the Lanczos results from Ref. [33] (error bars are not shown).

The mobility edge.—Finally, we can observe the transition at different energy windows by varying $\beta = 1/T$ in Eq. (3) of our NLC calculation, thus probing states at a given energy defined by the thermal ensemble. Following the same arguments as at $T = \infty$, we can obtain estimates for h_c at a given temperature or energy density. Figure 3 shows our estimates for various β values, with the scaled energy ϵ on the vertical axis: $\epsilon = (E - E_{\min})/(E_{\max} - E_{\min})$, where $E_{\min}$ and $E_{\max}$ are the lowest and highest energies in the energy spectrum. The shape of our estimates are very similar to those obtained in previous numerical calculations [32,33], along with the slight asymmetry expected around $\epsilon = 1/2$ [69]. As with the case at $T = \infty$, we find that our estimates are consistently higher than previous numerical calculations.

There is much debate on whether a mobility edge exists in the thermodynamic limit. Numerical results suggest the presence of such an edge [32,33,69], but there are also arguments against it [70]. While our phase diagram shows a similar shape as previous numerical studies, our analysis gives a lower bound for h_c, and hence it does not negate the claims of the absence of a mobility edge. If the transition actually occurs at a single h_c for all energies, the fact that our estimates are lower away from the center of the spectrum would indicate that much larger length scales would be needed to observe delocalization and that finite size effects would be much stronger in those regions.

Conclusions.—In conclusion, we have studied the MBL transition in the random field Heisenberg model using NLC expansions. We focus on the breakdown of the area law of entanglement in the eigenstates of the Hamiltonian. Our approach works directly in the thermodynamic limit and does not rely on any finite size scaling. By looking for signs of instability in the MBL phase, we are able to estimate a lower bound for the critical disorder in the thermodynamic limit. At all energies examined, our h_c estimates are consistently higher than those found in finite size studies. This implies that numerical methods which look for the full onset of thermalization tend to overestimate the extent of the MBL phase, which actually becomes unstable earlier but only at much longer length scales. Near the transition, finite size effects are significant, and hence caution must be taken when relating to the infinite system.

Our result can be readily verified by cold atom experiments, which are able to present very well characterized systems [28–31]. If the 1D random field Heisenberg model is experimentally realized, measurements of the critical disorder for large systems should lie above our estimate. We may also extend our result to other similar models of the disorder driven MBL transition, where delocalization also occurs over a long length scale [67,68], and suggest that the true critical point would be higher than finite size scaling estimates from small systems. Also of interest are quantum chaotic Wannier-Stark systems [71,72], which are experimentally accessible and possess a localization-delocalization transition in the absence of disorder.

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