Many-body localization in the thermodynamic limit

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We use thermalization indicators and numerical linked cluster expansions to probe the onset of many-body localization in a disordered one-dimensional hard-core boson model in the thermodynamic limit. We show that after equilibration following a quench, the momentum distribution indicates a freezing of one-particle correlations at higher values than if the system were in thermal equilibrium. The position of the delocalization to localization transition, identified by the breakdown of thermalization with increasing disorder strength, is found to be consistent with the value from the level statistics obtained via full exact diagonalization of finite chains. Our results strongly support the existence of a many-body localized phase in the thermodynamic limit.

Since the first quantitative discussion of localization by Anderson in 1958 [1], a large number of experiments have revealed phenomena governed by localization physics, see e.g., Refs. [2, 3]. In the absence of interactions, destructive interference due to scattering off impurities is responsible for localization [1]. What happens in the presence of interactions has remained an open problem whose exploration has become an active area of research over the past few years. For weak interactions, perturbative arguments support the existence of localized phases [4–7]. For strong interactions, on the other hand, numerical studies have found signatures of many-body localization and explored its implications [8–20]. Nonetheless, it remains a challenge to conclusively establish that, in the presence of strong interactions, the delocalization to localization transition occurs at finite disorder strength in the thermodynamic limit.

The signatures of localization in experiments are mostly dynamical in nature, e.g., measurements of the conductivity [3]. Theoretically, it is difficult to study dynamical properties [3]. So, to identify many-body localized phases, it is common to use the statistics of the energy level spacing instead (see, e.g., [8, 11]). Poissonian level statistics is expected for localized phases, whereas Wigner-Dyson statistics is expected for delocalized ones. Equally accessible to experimental and theoretical studies is a remarkable but less explored signature of many-body localization – when taken far from equilibrium, isolated localized systems do not relax to thermal equilibrium [21].

Relaxation dynamics and thermalization in isolated many-body quantum systems is a very active area of current research on its own [22–24]. There is growing evidence that generic many-body quantum systems thermalize after being taken far from equilibrium [25–30], and that this is a consequence of eigenstate thermalization [25–27, 31–41]. That is, thermalization results from the fact that, for observables of interest, individual eigenstates of the Hamiltonian already exhibit thermal properties [25, 31, 32]. This can be pictured as the system effectively acting as its own bath. Such a picture is expected to breakdown in a many-body localized phase as different parts of the system cannot communicate with one another, i.e., the localized phase cannot be ergodic [21]. Evidence of the breakdown of eigenstate thermalization [11] and thermalization [11, 42] in many-body localized phases have been found in numerical calculations in finite systems.

Here, we study quantum quenches in disordered isolated systems in the thermodynamic limit. By a quantum quench it is meant that the initial state is stationary with respect to an initial Hamiltonian, which is suddenly changed to a new (time-independent) Hamiltonian. The latter then drives the (unitary) dynamics of the system. We are interested in the time average of observables (say, $\hat{O}$) after the quench. They can be calculated as $O(\tau) = \text{Tr}[\rho(\tau)\hat{O}] = \text{Tr}[\hat{\rho}(\tau)\hat{O}] \equiv \text{Tr}[\hat{\rho}_{\text{DE}}\hat{O}] = O_{\text{DE}}$, where $(\tau) = \lim_{\tau' \to \infty} 1/\tau' \int_{0}^{\tau'} d\tau \langle \cdot \rangle$ indicates the infinite time average, $\hat{\rho}(\tau)$ is the density matrix of the time-evolving state, and $\hat{\rho}_{\text{DE}} \equiv \hat{\rho}(\tau)$ is the density matrix of the so-called diagonal ensemble (DE) [25]. To obtain results in the thermodynamic limit, we use a recently introduced numerical linked cluster expansion (NLCE) for the DE [30, 43]. NLCEs for systems in thermal equilibrium were introduced in Refs. [44, 45], and their implementation was discussed in Ref. [46]. When converged, NLCE calculations provide exact results in the thermodynamic limit. Thermalization, or the lack thereof, are established by comparing results for observables in the DE and in the grand-canonical ensemble (GE).

We focus on a system of impenetrable bosons in one-dimension (1D) with Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_D$, where

$$\hat{H}_0 = \sum_i \left[ -t(b_i^\dagger \hat{b}_{i+1} + \text{H.c.}) + V \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_{i+1} - \frac{1}{2} \right) \right]$$

(1)

is translationally invariant and $\hat{H}_D = \sum_i h_i(\hat{n}_i - \frac{1}{2})$ is the term with the disorder. $b_i^\dagger$ ($b_i$) creates (annihilates) a hard-core boson at site $i$, and $\hat{n}_i = b_i^\dagger b_i$ is the site number operator. $t$ stands for the hopping parameter, $V$ for the nearest neighbor interaction, and $h_i$ for the strength of the on-site disorder. In the spin language, $\hat{H}$ describes a spin-1/2 XXZ model in the presence of a random mag-
netic field in the $z$-direction. We select the random field to have a binary distribution with equal probabilities for $h_i = \pm h$. This model has been recently motivated in the context of ultracold bosons in optical lattices [17].

We first check whether $\hat{H}$ supports a many-body localized phase (as argued in Ref. [17]) and, if it does, the value of the disorder strength at which such a phase appears. We focus on $V = 2t$ (which is the Heisenberg point in the spin model) and set $t = 1$ as our unit of energy. As a first indicator of many-body localization, we study the averaged ratio of the smaller and the larger of two consecutive energy gaps, $r_n = \min(\delta_{E_n}^+ - \delta_{E_n}^-)/\max(\delta_{E_n}^+ - \delta_{E_n}^-)$, where $\delta_{E_n} = E_{n+1} - E_n$ is the difference between adjacent energy levels in the spectrum. The averaged ratio $r$ is obtained by averaging $r_n$ over the central half of the spectrum for a given disorder configuration, and then averaging over disorder configurations. In the delocalized phase one expects $r \approx 0.5359$ and in the localized one, $r \approx 0.3863$, corresponding to the results for the Wigner-Dyson and Poissonian distributions [47], respectively.

Figure 1 shows the ratio $r$ as a function of the strength of the random field $h$ for three system sizes. One can see that there is a transition from a delocalized to a localized phase with increasing disorder strength, and that it sharpens with increasing system size. From the delocalized side, with increasing $h$, the curves for different system sizes meet in the vicinity of $h = 3.5$, suggesting that the critical $h_c \approx 3.5$. Remarkably, for the same model but with continuous disorder, an earlier study estimated the transition to also be at $h_c \approx 3.5$ [10].

Now that we have an idea of the disorder strengthes that correspond to the ergodic and many-body localized phases, we proceed to study quantum quenches into both regimes. We take the initial state to be in thermal equilibrium at some temperature $T_I$ for $\hat{H}_I$ with parameters $t_I = 0.5$, $V_I = 2.5$, and $h_j = 0$ for all $j$, i.e., the initial state is homogeneous. After the quench, $\hat{H}$ has $t = 1$, $V = 2.0$, and different values of $h \neq 0$ (as in Fig. 1). In all our calculations, $\mu = 0$ before and after the quench. NLCEs for the diagonal ensemble allow one to compute the infinite time average of observables in the thermodynamic limit for lattice systems evolving unitarily [30, 43]. The conceptual NLCE development introduced in this work is the ability to deal with systems with disorder.

In translationally invariant systems, NLCEs allow one to calculate the expectation value of an extensive observable per lattice site in the thermodynamic limit, $\mathcal{O}$, as a sum over the contributions from all clusters $c$ that can be embedded on the infinite lattice: $\mathcal{O} = \sum_c M(c) \times W_{\mathcal{O}}(c)$, where $M(c)$ is the multiplicity of $c$, defined as the number of ways per site in which cluster $c$ can be embedded on the lattice. $W_{\mathcal{O}}(c)$ is the weight of $\hat{O}$ in cluster $c$, which is calculated recursively using the inclusion-exclusion principle $W_{\mathcal{O}}(c) = \mathcal{O}(c) - \sum_{c' \subset c} W_{\mathcal{O}}(c')$, where $\mathcal{O}(c) = \text{Tr}[\hat{O}\hat{\rho}_c]$ is computed using full exact diagonalization, with $\hat{\rho}_c$ being the density matrix relevant to the calculation [e.g., of the grand-canonical ensemble (GE) or the diagonal ensemble (DE)] in cluster $c$ [30, 43].

Such an expansion cannot be applied to systems in which translational symmetry is broken, e.g., by disorder. However, a disorder average that restores an exact translational invariance enables once again the use of
NLCEs. The two crucial points that make that possible are: (i) the linear character of the equations defining the linked cluster expansion (reproduced above), so that disorder average can be computed with the NLCE summation process, and (ii) the use of binary disorder that, after averaging over all possible disorder realizations, allows us to restore the translational symmetry (and also particle-hole symmetry) of $H_0$. Hence, all we need to do in our calculations is replace $O(c) = \text{Tr}[\hat{O}\rho_c]$ for the translationally invariant case by:

$$O(c) = \left\langle \text{Tr}[\hat{O}\rho_c]\right\rangle_{\text{dis}},$$

where $\langle \rangle_{\text{dis}}$ represents the disorder average. Having to compute this additional average reduces our site based linked cluster expansion from a maximum of 18 sites for translationally invariant systems [30, 43] to 14 sites here. We define $O_{\text{ens}}^{\text{ens}}$ as a sum over the contributions of clusters with up to $l$ sites, where “ens” could be DE or GE. The temperature used in the GE calculations to describe the system after the quench is determined from a comparison of the linked cluster expansion from a maximum of 18 sites for $h=1.0$ to 14 sites here. We report results for values of $T_I$ for which $E_{14}^{\text{DE}}$ and $E_{14}^{\text{GE}}$ are converged within machine precision (see Ref. [48]).

In Fig. 2, we report the initial momentum distribution of a system with $T_I = 2$ and for different values of $h$ after the quench. The DE and GE results for the momentum distribution function for $h = 0.6$ and 1 ($h < h_c$) are indistinguishable from each other, while for $h = 4$ and 6 ($h > h_c$) are very different from each other. Remarkably, the results that are close to each other for $h > h_c$ are those from the DE. The contrast between the DE and GE results in this regime makes apparent that there is more coherence in the one-particle sector after equilibration than if the system was in thermal equilibrium ($m_k^{\text{DE}} > m_k^{\text{GE}}$). The system “remembers” one-particle correlations from the initial state. This has also been seen in quasi-periodic systems [49]. It is easy to understand in the limit of very strong disorder, where $H = \sum_i h_i (\hat{n}_i - \frac{1}{2})$, and, in the Heisenberg picture, $\hat{b}_i(\tau)\hat{b}_j(\tau) = \exp[i(h_i-h_j)\tau/\hbar]\hat{b}_i(0)\hat{b}_j(0)$. A disorder average over $h_i, h_j$ with each being $\pm$ with equal likelihood reveals that, for a half-filled system, $m_k^{\text{DE}} = 1/4 + m_k(\tau = 0)/2$. Strikingly, a very strong freezing of correlations can already be seen right after entering the many-body localized phase. The results for the kinetic energy, reported in the inset in Fig. 2, provide evidence of the robustness of these findings.

To discern which of the differences between the DE and GE seen in Fig. 2 are due to insufficient convergence of the NLCE and which of them are expected to survive in the thermodynamic limit, we calculate the following two differences

$$\delta(m)_l = \frac{\sum_k |(m_k)^{\text{DE}} - (m_k)^{\text{GE}}|}{\sum_k |(m_k)^{\text{GE}}|},$$

which allows us to quantify the difference between the DE and the GE, and

$$\Delta(m_{\text{ens}})_l = \frac{\sum_k |(m_k)^{\text{ens}} - (m_k)^{\text{ens}}|}{\sum_k |(m_k)^{\text{ens}}|},$$

which allows us to estimate the convergence of the NLCE calculations [30]. $\delta(K)_l$ and $\Delta(K_{\text{ens}})_l$ follow straightforwardly from Eqs. (3) and (4), respectively, by removing the sums and replacing $m_k \rightarrow K$. For the GE calculations when $T_I > 1$, $(m_k)^{\text{GE}}$ and $K^{\text{GE}}$ are converged within machine precision (see Ref. [48]).

![Figure 3](image-url)
Results for $\delta(m)_l$, $\delta(K)_l$, $\Delta(m^{DE})_l$, and $\Delta(K^{DE})_l$ vs $l$ are reported in Figs. 3(a)–3(d), respectively, for six values of $h$. They show that: (i) The momentum distribution function (a nonlocal quantity) and the kinetic energy (a local quantity) exhibit qualitatively similar behavior. (ii) For $h \gtrsim 3.5$, $\delta(m)_l$ and $\delta(K)_l$ do not change with increasing $l$, and are much larger than $\Delta(m^{DE})_l$ and $\Delta(K^{DE})_l$, i.e., they are expected to remain in the thermodynamic limit. This support the existence of many-body localization in the thermodynamic limit. (iii) For $h \lessgtr 3.0$, $\delta(m)_l$ and $\delta(K)_l$ decrease with increasing $l$, and are of the same order of magnitude as $\Delta(m^{DE})_l$ and $\Delta(K^{DE})_l$ (which also decrease with increasing system size). Hence, the differences between those observables in the DE and the GE are expected to vanish in the thermodynamic limit, i.e., those values of $h$ belong to the ergodic phase. In this phase, $\delta(m)_l$ and $\delta(K)_l$ behave exactly as in systems without disorder $[30]$. (iv) $\Delta(m^{DE})_l$ and $\Delta(K^{DE})_l$ in Figs. 3(c)–3(d) show that the NLCE convergence errors are largest in the region where the system transitions between ergodic and localized.

In order to better pin down the transition point between the ergodic and many-body localized phases, in Fig. 4(a) we plot $\delta(m)_l$ vs $l$ in the vicinity of $h = 3.5$. For $h \geq 3.6$, we see that $\delta(m)_l$ seems to saturate to a finite value that is larger than $\Delta(m^{DE})_{13}$, suggesting that the system is many-body localized for $h \geq 3.6$. The transition between ergodic and many-body localized can occur for smaller values of $h$ as, for larger values of $l$, the plots for $\delta(m)_l$ may saturate to a constant value. However, we expect that $h_c \approx 3.5$ in the vicinity of this disorder strength we see that $\delta(m)_l$ and $\Delta(m^{DE})_{l-1}$ are very close to each other for the largest system sizes studied.

We should stress that, for $T_I > 2$, we do not find indications that $h_c$ increases significantly with increasing $T_I$. In general, it is expected that as one increases the mean energy density after the quench (which is exactly what increasing $T_I$ does in our case) the transition point between the delocalized and localized phases should move towards larger disorder strengths $[15]$. In our system of interest, probably a lower $T_I$, for which our GE results would not be converged within machine precision, is needed to observe that effect.

In summary, we have studied quantum quenches in the thermodynamic limit in an interacting model with binary disorder. This was possible by extending the NLCE approach introduced in Ref. $[30]$ to solve problems with binary disorder. We have shown that for quenches starting in a delocalized phase, a freezing of correlations in the steady state after the quench can occur right after entering the many-body localized phase. We located the critical value of the transition between the ergodic and many-body localized phase using a quantum chaos indicator (the average ratio between consecutive energy gaps) in finite systems and the difference between NLCE predictions for observables in the DE and the GE after quantum quenches. The values of $h_c$ were found to be consistent in those two methods. The small convergence errors of NLCE for $h > h_c$ strongly support that the many-body localized phase will occur in the thermodynamic limit.

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[1] P. W. Anderson, Phys. Rev. B 109, 1492 (1958).
[2] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. 57, 287 (1985).
[3] B. Kramer and A. MacKinnon, Rep. Prog. Phys. 56, 1469 (1993).
[4] L. Fleishman and P. W. Anderson, Phys. Rev. B 21, 2366 (1980).
[5] B. L. Altshuler, Y. Gefen, A. Kamenev, and L. S. Levitov, Phys. Rev. Lett. 78, 2803 (1997).
[6] I. V. Gornyi, A. D. Mirlin, and D. G. Polyakov, Phys. Rev. Lett. 95, 206603 (2005).
[7] D. Basko, I. Aleiner, and B. Altshuler, Annals of Physics 321, 1126 (2006).
[8] V. Oganesyan and D. A. Huse, Phys. Rev. B 75, 155111 (2007).
[9] M. Žnidarič, T. Prosen, and P. Prelovšek, Phys. Rev. B 77, 064426 (2008).
[10] A. Pal and D. A. Huse, Phys. Rev. B 82, 174411 (2010).
[11] E. Khatami, M. Rigol, A. Relano, and A. M. Garcia-Garcia, Phys. Rev. E 85, 050102(R) (2012).
[12] J. H. Bardarson, F. Pollmann, and J. E. Moore, Phys. Rev. Lett. 109, 017202 (2012).
[13] R. Vosk and E. Altman, Phys. Rev. Lett. 110, 067204 (2013).
Convergence of NLCEs for the DE and the GE

NLCEs, when converged, give exact results in the thermodynamic limit. Here, we check the convergence of the calculations. We define the difference

\[ \Delta(O^{\text{ens}})_l \equiv \frac{|O^{\text{ens}}_l - O^{\text{ens}}_{l+1}|}{|O^{\text{ens}}_{l+1}|} \]

where \( O \) is either the kinetic energy \( K \) or the energy \( E \). For the momentum, we define

\[ \Delta(m^{\text{ens}})_l \equiv \frac{\sum_k |(m_k)^{\text{ens}}_l - (m_k)^{\text{ens}}_{l+1}|}{\sum_k |(m_k)^{\text{ens}}_{l+1}|} \]

where \( m_k \) is the momentum distribution function. In all cases, "ens" refers to either the diagonal ensemble (DE) or the grand-canonical ensemble (GE).

In order to determine the initial temperature \( T_I \) for which the various observables calculated using NLCEs in the DE and GE are well converged, we plot \( \Delta (E^{\text{ens}})_1 \) in Fig. 5(a), \( \Delta (K^{\text{ens}})_1 \) in Fig. 5(b), and \( \Delta (m^{\text{ens}})_1 \) in Fig. 5(c) as a function of \( T_I \) for the same set of quenches as in Fig. 3 in the main text. Figure 5 shows that, with increasing \( T_I \), \( \Delta (E^{\text{ens}})_1 \), \( \Delta (K^{\text{ens}})_1 \), \( \Delta (m^{\text{ens}})_1 \) decrease and become zero within machine precision for \( T_I \gtrsim 2.0 \).

We therefore expect that, within the cluster sizes accessible to us, \( E \), \( K \), and \( m \) in the GE have converged to the thermodynamic limit results for \( T_I \gtrsim 2.0 \). In the DE, however, only the energy [Fig. 5(a)] converges within machine precision. As evident from Figs. 5(b) and 5(c), the error can only be reduced by considering larger system sizes.

Critical disorder strength at higher temperature

In Figure 6, we show the equivalent of Fig. 4 in the main text but for higher initial temperatures. As mentioned there, a higher temperature is expected to increase the value of the critical strength required for the localized phase to appear. However, for the temperatures at which

Supplementary Materials:
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FIG. 5. (Color online) Results for: (a) $\Delta(E)_{13}$, (b) $\Delta(K)_{13}$, and (c) $\Delta(m)_{13}$ as a function of $T_I$ for the same set of quenches as in Fig. 3 in the main text. Open (filled) symbols depict the relative differences in the DE (GE). In all panels, the GE results appear converged within machine precision for temperatures $T_I \gtrsim 2$. For the DE, only the energy (a) converges within machine precision.

TABLE I. Effective temperatures used in the GE calculations

| $T_I$ | $h = 0.6$ | $h = 1.0$ | $h = 3.0$ | $h = 3.5$ | $h = 4.0$ | $h = 6.0$ |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| 2.0   | 2.996     | 3.482     | 9.900     | 12.558    | 15.635    | 32.095    |
| 10.0  | 14.894    | 17.590    | 51.858    | 65.850    | 82.005    | 168.226   |
| 100.0 | 149.283   | 177.563   | 531.698   | 675.640   | 841.738   | 1727.657  |

our NLCEs for the energy converge within machine precision, we do not observe any significant difference between the results for $T_I = 2$, 10, and 100. This is possibly because $T_I = 2$ is already too high to see this effect. The effective temperature after the quench are reported in Table I.
FIG. 6. (Color online) The equivalent of Fig. 4 in the main text for $T_I = 10$ (left) and $T_I = 100$ (right). For $h \geq 3.6$, $\delta(m)$ vs $l$ [(a) and (c)] appears to converge to a nonzero value with increasing system size. Furthermore, the convergence errors [estimated by $\Delta(m_{DE})$, see panels (b) and (d)] are smaller than the $\delta(m)$ differences for those values of $h$. These results are very similar to those for $T_I = 2$ reported in the main text.