How a small quantum bath can thermalize long localized chains

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We investigate the stability of the many-body localized (MBL) phase for a system in contact with a single ergodic grain, modelling a Griffiths region with low disorder. Our numerical analysis provides evidence that even a small ergodic grain consisting of only 3 qubits can delocalize a localized chain, as soon as the localization length exceeds a critical value separating localized and extended regimes of the whole system. We present a simple theory, consistent with the arguments in [Phys. Rev. B 95, 155129 (2017)], that assumes a system to be locally ergodic unless the local relaxation time, determined by Fermi’s Golden Rule, is larger than the inverse level spacing. This theory predicts a critical value for the localization length that is perfectly consistent with our numerical calculations. We analyze in detail the behavior of local operators inside and outside the ergodic grain, and find excellent agreement of numerics and theory.

Introduction — The phenomenon of Many-Body Localization (MBL) [1–15] has challenged our ideas on thermalization and the applicability of thermodynamics. It is hence important to determine the precise conditions for the stability of the MBL phase. Whereas in the original works [3, 4], the spatial dimension $d$ did not play a central role, the rigorous treatment of Griffiths regions of low disorder [16] in [17] relies on $d = 1$, not for technical but for conceptual reasons. More generally, it is now well understood that there is a huge variety of systems where thermalization is effectively inhibited locally and only rare Griffiths regions can, possibly, restore ergodicity [18, 19]. This applies in particular to quasi-localization [20–26], classical disordered models [27, 28] or even glasses [29, 30]. It is also believed that Griffiths regions drive the transition from MBL to ergodicity [31–36]. This raises the fundamental issue of understanding the effect of a Griffiths region, in practice an ergodic grain or imperfect bath, on a localized system. We outline a very simple theory: local ergodicity characterized by the Eigenstate Thermalization Hypothesis (ETH) [37–43] is taken as the default option, and a degree of freedom is interpreted as localized if the local relaxation time would be larger than the inverse level spacing. In [44] a more microscopically motivated version of this theory was proposed leading to precisely the same conclusions. The main result is the instability of MBL if the bare localization length is larger than a critical value [45]. This predicted instability implies that a single, sufficiently large, interacting, ergodic grain thermalizes the whole system if the localization length in the localized part of the system is large enough. This striking conclusion is counter-intuitive, and it has often been suggested to us, e.g. [46], that localization should prevail when the number of a priori localized degrees of freedom clearly exceeds the number of degrees of freedom in the bath. In this letter, we investigate this aspect, using a setup where the ergodic grain is considerably smaller than the surrounding localized system, namely 3 versus 13 spins. All results of our numerical analysis confirm the simple theory, leading to thermalization of the chain by a small ergodic grain.

Theoretical predictions — Let us consider a system of size $L = L_{\text{loc}} + L_0$ containing an ergodic grain (or bath) of size $L_0$ interacting with a fully localized chain of size $L_{\text{loc}}$. The full system is described by the Hamiltonian $H = H_0 + H_{\text{loc}} + H_{\text{id}}$. We assume that the bath Hamiltonian $H_0$ satisfies the eigenstate thermalization hypothesis (ETH). $H_{\text{loc}}$ describes an Anderson insulator in the basis of localized integrals of motion (LIOMs) [5, 15, 47–54], and $H_{\text{id}}$ couples the bath locally to the LIOMs. A LIOM at distance $\ell$ from the bath is connected to the bath by a coupling strength $g_\ell := g_0 e^{-\ell/\xi} = g_0 e^{-\xi/\ell}$ reminiscent of the interaction of an MBL system with the grain, where $\alpha = e^{-1/\xi}$ and where $\xi$ denotes the localization length (in lattice units); cf. Fig. 1 and Eq. (5) for the model used in the numerics.

ETH provides an ansatz for the matrix elements of a local operator $A$ in an ergodic system. Let $E, E'$ label eigenstates with energy density $\epsilon_0 = E/L \sim E'/L$, and let $\langle A \rangle_{\epsilon_0} = 0$ (ensemble average in an equilibrium state at $\epsilon_0$). Below we always let $\epsilon_0$ correspond to maximal entropy and we drop $\epsilon_0$ from the notation. Then, ETH amounts to [42]

$$
\langle E' | A | E \rangle = \sqrt{\delta f(\omega)} \eta_{E, E'} (E \neq E')
$$

(1)

with $\delta$ the many-body level spacing at density $\epsilon_0$, $\omega =$...
$E - E'$ the energy difference, $\eta_{E,E'}$ random numbers with zero mean and unit variance and $f(\omega)$ a smooth function that can be related to a time-dependent correlation function and that satisfies the sum rule \( \int d\omega |f(\omega)|^2 = \langle A^\dagger A \rangle_{\text{eq}} \sim 1 \). For local $A$, $f(\omega)$ is roughly supported on intervals of size $\Delta$, where $\Delta$ can be interpreted as the typical rate at which local quantities equilibrate [42, 55, 56] [57]. Obviously, the ansatz (1) only makes sense if $\Delta \gg \delta$ (otherwise (1) conveys no information), which we use as a consistency condition that will be invoked below in a crucial way. Let us give a relevant example of how to determine $\Delta$: take one LIOM with field $h$ coupled to an ergodic system (e.g. our ergodic grain) via a weak coupling term of strength $g$. Then, under some mild conditions, Fermi's Golden Rule predicts $f(\omega)$ of that LIOM in the combined system to have principal peaks at the Bohr frequencies $\pm 2\hbar$ with widths of order $\Delta = g^2 / \epsilon$, for some local energy scale $\epsilon$ characterizing the bath, see e.g. [44].

Now, we couple LIOMs $i = 1, \ldots, L_{\text{loc}}$ to the bath (cf. Fig. 1) with couplings $g_i = g_0 \alpha^i$ and compute the local rates $\Delta_i$ as in the example above, namely $\Delta_i \sim \alpha^{2i} g_0^2 / \epsilon$. Now we assume that ETH is valid as long as it is not inconsistent, i.e. as long as $\delta \ll \Delta_i$ for all $i \leq L_{\text{loc}}$. This central assumption will lead to striking consequences, presented below. Verifying these consequences is the main point of the paper. We conjecture hence that ETH for the full system is valid if and only if

\[
\langle g_0^2 / \epsilon \rangle \alpha^{2L_{\text{loc}}} \geq W 2^{-L},
\]

where we put $\delta = W 2^{-L}$ with $W = \epsilon_0 L$ the spectral width. Neglecting all non-exponential dependence on the lengths $L_{\text{loc}}, L_b$, the condition for full ETH becomes (leading order in $L_b \gg 1$)

\[
L_{\text{loc}} \leq L_c = \frac{L_b \log 2}{\log \alpha - 2 - \log 2}.
\]

The most striking consequence of this analysis is that $L_c = \infty$ if $\alpha > \alpha_c = 1 / \sqrt{2}$ (and $L_b$ is not too small). That is: a small bath is capable of thermalizing an arbitrary number of LIOMs. This is a sharp prediction that can be tested numerically by studying the validity of ETH as a function of $\alpha$.

Let us add a more quantitative prediction of the theory: The local rates $\Delta_i$ correspond to an effective dimension $d_i = \Delta_i / \delta$, i.e. the number of eigenstates $|E_i\rangle$ over which $A_i|E\rangle$ is spread out, according to (1), for a local operator $A_i$ at site $i$. Then our theory predicts that

\[
d_i \approx 2^{L_{\text{therm}}} \alpha^{2i}, \quad L_{\text{therm}} = L_b + \min(L_{\text{loc}}, L_c),
\]

as long as $d_i \geq 1$, and setting $d_i = 1$ otherwise, corresponding to localization at site $i$. Here, $L_{\text{therm}}$ is the length of the thermal region and for $\alpha > \alpha_c$, we simply have $L_{\text{therm}} = L$. In the rest of this letter, we present the several numerical results that demonstrate the accuracy of the above picture for numerically accessible system sizes.

**Model** — We start from a simplified model of an ergodic grain coupled to localized spins, as depicted on Fig. 1, where the Hamiltonian of the ergodic grain is given by a random matrix $R$ drawn from the GOE ensemble: $R = (1/2) (A + A^T) \in \mathbb{R}^{2^L_b \times 2^L_b}$ where $A_{ij} = \text{norm}(0,1)$ with norm(0,1) random numbers drawn from a normal distribution with zero mean and unit variance.

Now, we can specify the Hamiltonian for our model for an ergodic grain of size $L_b$ and a set of LIOM’s on sites $0, \ldots, L_{\text{loc}} - 1$.

\[
H = R + \sum_{i=0}^{L_{\text{loc}}-1} \frac{h_i}{2} \sigma_i^z + \sum_{i=0}^{L_{\text{loc}}-1} \frac{g_0 \alpha^i}{4} \sigma_i^x \sigma_{i+1}^x.
\]

The system has no conservation laws except energy and the total Hilbert space dimension is $\dim(H) = 2^{L_b}$. We restrict the size of the ergodic grain to $L_b = 3$ (on sites $-3, -2, -1$, hence $\sigma_{-1}^x$ is a bath operator). For a more accurate correspondence of the LIOMs to a generic MBL system, we would need to include interactions of the type $\sigma_i^z \sigma_{i+1}^z$. For simplicity, we omit those interactions, thus making our localized chain basically an Anderson Insulator (AI). This simplification does not change the physics, since anyhow the bath coupling makes the full system truly interacting. Our theory is hence not in conflict with the fact that one can construct AIs with arbitrarily large localization lengths.

The onsite fields $h_i$ are drawn from a random box distribution $[1 - W, 1 + W]$, $W = 0.5$. The shift of the
box distribution by $1$ is not necessary but reduces finite size effects. We have checked carefully that a symmetric distribution around $0$ yields similar results. In all our experiments, $L_b = 3$, $\beta = 0.3$, $g_b = 1$. We have selected these values so as to obtain the cleanest results with the smallest bath size and the smallest coupling constant $g_b$, however our results remain qualitatively similar if any of these three parameters is varied (with $L_b \geq 3$). In order to infer the behavior of the system in the thermodynamic limit, we vary the number $L_{\text{loc}}$ of localized spins coupled to the bath, with $L_{\text{loc}} \leq 13$. For $L_{\text{loc}} = 13$, the coupling strength of the last spin is $g_{\text{min}} = g_0\alpha^{12}$. For $\alpha = 0.8 > \alpha_c$, the direct coupling to the bath is $0.8^{12} \approx 0.068$ and does not suffice to trivially thermalize the last few spins (cf. Supplemental Material). Thus, for such values of $\alpha$, the thermalization of the last spins results from highly non-trivial effects involving all spins in between.

**Spectral statistics** — A powerful and very general measure of ergodicity of quantum systems are the statistical properties of its energy spectrum, typically studied in the center of the spectrum. The gap ratio\cite{6,7} $r = \min(\Delta E_k, \Delta E_{k+1})/\max(\Delta E_k, \Delta E_{k+1})$ with $\Delta E_k = E_{k+1} - E_k$ is Poisson distributed for localized systems and GOE distributed for ergodic ones, as an account of level repulsion \cite{58}. In Fig. 2, we show the average of $r$ as a function of $\alpha$ for various system sizes $L$. A clear tendency towards GOE statistics for $\alpha \geq 0.7$ and towards Poisson statistics for $\alpha \leq 0.7$ is visible, consistently with the theoretical value for $\alpha_c \approx 0.7071$. It is important to note that in the supercritical regime, the increase of $\langle r \sigma_z^2 \rangle$ with $L$ is due to the addition of increasingly weakly coupled spins. To get a more detailed picture near the transition, we show the full distribution of $r$ for $\alpha = 0.6, 0.7, 0.8$: For $\alpha = 0.6, 0.7$ we observe a clear drift towards Poisson statistics as the system sizes increases, while no deviation from the GOE statistics is observed at $\alpha = 0.8$ up to $L = 16$ \cite{59}.

**Local magnetizations** — A direct test of the validity of ETH is furnished by the diagonal values of a local operator (here $\sigma_z^2$) in the eigenbasis of the Hamiltonian: $\langle E | \sigma_z^2 | E \rangle$. In a localized system, the distribution of $\langle E | \sigma_z^2 | E \rangle$ is sharply bimodal with peaks at $\pm 1$, since the LIOMs are small perturbations of the bare spins $\sigma_z^2$. For an ergodic system, the distribution is sharply peaked around the thermal value (here: $0$), with variance scaling \cite{60,61} as $1/d_i$ with $d_i$ the effective dimension, as computed in Eq. (4). To test this, we show in Fig. 3 (top) the standard deviation over disorder and all eigenstates $|E\rangle$ in a small window at maximal entropy of the expectation values $\langle E | \sigma_z^2 | E \rangle$, as a function of site index $-3 \leq i < L_{\text{loc}}$ for $\alpha = 0.6 < \alpha_c$ and $\alpha = 0.8 > \alpha_c$. At $\alpha = 0.6$, we observe that the standard deviation goes down slightly for $i < 0$ as we start increasing $L$ but saturates quickly to a constant value. This indicates that the first spins near the bath are thermalized and increase the effective dimension for local operators in the bath, while spins further away, at $i > L_{\text{loc}}$, remain localized and do not affect the effective dimension. For $\alpha \geq 0$, the standard deviation tends to its maximal value $1$ as the operator moves away from the bath, consistently with the fact that only the closest spins get thermalized. The very good data collapse at large $L$ indicates that stationary values have been reached. The situation is strikingly different at $\alpha = 0.8$: at any fixed distance $i$ from the bath, the standard deviation decreases as the total length $L$ increases, because all spins contribute to the effective dimension. On the other hand, for fixed $L$, the standard deviation always increases as one moves away from the bath (i.e. as $i$ increases). This is fully consistent with the decreasing effective dimension predicted in (4) and it should hence not be interpreted as some sort of “imperfect thermalization”. Finally, it is instructive to compare the standard deviation of the last spin at different $L$, i.e. the endpoints of the curves: these endpoints move down with increasing $L$. Thus, the last spins become more and more delocalized, even though they also move further away from the original bath.

This picture is even clearer in the full distribution of $\langle E | \sigma_z^2 | E \rangle$ shown for $L = 16$ for a subset of sites $i$ and $\alpha = 0.6, 0.8$ in Fig. 3 (bottom). At $\alpha = 0.6$, the distribution of all but the first few spins become strongly bimodal with peaks as $\pm 1$, indicating that spins far away from the bath are indeed not thermalized. In contrast, for $\alpha = 0.8$, we see a progressive broadening of the dis-
distribution as \( i \geq 0 \) increases but no signs of bi-modality, confirming thus the above conclusion. Interestingly, we observe that for all thermalized spins, the distribution departs from a gaussian due to the presence of heavier tails compared to gaussian distributions. This phenomenon has recently been observed in ergodic systems at moderate values of disorder where the dynamics is expected to be sub-diffusive [55, 62].

Participation entropy — Up to here, we have defined the “effective dimension” \( d_\ell \) of the Hilbert space only via the spectral function \( f(\omega) \). Let us introduce now the participation Rényi entropies \( S_\alpha \) to obtain a more direct definition:

\[
S_\alpha = \frac{1}{1-\alpha} \log \sum_E \langle |E_0| \sigma_i^x |E\rangle^{\alpha}.
\]  

with \( E_0 \) a state of energy density \( \epsilon_0 \) (at maximal entropy). Here, we will focus on the second Rényi entropy \( S_2 \). Before taking the logarithm, this quantity is analogous to the inverse participation ratio in one-particle localization[63]. For thermal systems at maximal entropy, \( S_2 \sim L \log 2 \) while for localized systems \( S_2 \sim \text{const.} \) as a function of the total size \( L \). In general, using the ETH (1), we find \( S_2 = -\log(\delta \int d\omega |f(\omega)|^4) \). If now \( f \) is mainly supported on a set of size \( \Delta_\ell \) and we use the sum-rule \( \int d\omega |f(\omega)|^2 \sim 1 \) (independent of \( L \)), then we find \( S_2 \approx \log(\Delta_\ell/\delta) \), which indeed equals \( \log d_\ell \) by our definition of \( d_\ell \). By comparison with (4) the theory predicts \( S_2 \sim \log(2) L_{\text{therm}} - 2 \log(\alpha)/i, \) (as long as \( S_2 \geq 0 \)).

We test these predictions for \( \alpha = 0.6 < \alpha_c \) and \( \alpha = 0.8 > \alpha_c \) in Fig. 4. Our results confirm the behavior that was already commented in the section on local magnetizations. In particular, at \( \alpha = 0.6 \), see Fig. 4 (top), we observe that \( S_2 \) first decreases linearly for small \( i \geq 0 \) then saturates to a constant value, because \( L_{\text{therm}} \) saturates to \( L_\ell \). The behavior of \( S_2 \) for a given site is plotted as a function of the total length in the right panels of Fig. 4: \( S_2 \) saturates to a constant value at all sites. For \( \alpha = 0.8 \) instead, \( S_2 \) increases linearly with system size at all sites \( i \), and decreases linearly with \( i \) for a given size \( L \); since the decrease with \( i \) is slower than the increase with system size, all spins can be thermalized for arbitrary large system sizes. The evolution of \( S_2 \) at a given site as a function of \( L \) shows a linear increase with a slope close to \( \log(2) \) as predicted theoretically.

Entanglement entropy — Finally, to have a more direct measurement of the thermalization of the last spins, we compute the entanglement entropy (EE) of the last four spins together for an eigenstate in the middle of the spectrum. If the last four LIOMs remain localized the EE should remain close to 0, and should converge to 0 as \( L \) is increased. Instead, if they are thermalized, the EE should approaches its maximal value \( 4 \log(2) \). The results are depicted on Fig. 5. In the left panel, we clearly see the trend that, for \( \alpha \lesssim 0.7 \), the the value of the EE decreases to 0, while it increases to \( 4 \log(2) \) for \( \alpha \gtrsim 0.7 \). This is all the more remarkable since the 4 last 1-bits are increasingly far away from the bath with increasing system size. A full distribution is plotted on the right panel for \( \alpha = 0.6, 0.8 \) at various lengths, confirming this trend.

Conclusion — We have demonstrated that a small ergodic grain can thermalize an arbitrary number \( L_{\text{loc}} \) of localized spins, provided the localization length of the localized spins exceeds the critical value \( 2/\log 2 \). This was achieved numerically by coupling spins with on-site disorder to a GOE system of dimension \( 8 = 2^3 \) with exponentially decreasing couplings. When the localization length is smaller than the critical value, the system drifts towards localization as more and more spins are added. When the localization is above the critical value, the sys-
SUPPLEMENTARY MATERIAL

Single LIOM — Here, we present additional numerical results for a single LIOM coupled to an ergodic grain of size \( L_0 = 3 \). Our main focus is to understand how large the direct coupling \( g \) has to be in order for the full system to be ergodic. In Fig. 6, we demonstrate that two limiting cases are reached: For large enough coupling \( g \gtrsim 0.5 \), the distribution of the adjacent gap ratio parameter \( r \) follows closely the GOE expectation, which means that the LIOM is well thermalized by the ergodic grain. In the case of completely decoupled LIOM and ergodic grain, the distribution is determined by a “folding” of two independent GOE spectra, denoted as GOE\(^2\) in Fig. 6. Clearly for small coupling strengths, \( g \lesssim 0.5 \), the distributions are quite close to this case and we conclude that if \( g = 0.1 \), the LIOM is not thermalized by the ergodic region. This strengthens our argument in the main text that for our longest chains and \( \alpha = 0.75, 0.8, 0.85 \), the last few spins are coupled so weakly to the ergodic region that they can not be trivially thermalized.

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