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Stability and instability towards delocalization in many-body localization systems

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We propose a theory that describes quantitatively the (in)stability of fully many-body localization (MBL) systems due to ergodic, i.e., delocalized, grains, that can be, for example, due to disorder fluctuations. The theory is based on the ETH hypothesis and elementary notions of perturbation theory. The main idea is that we assume as much chaoticity as is consistent with conservation laws. The theory describes correctly—even without relying on the theory of local integrals of motion (LIOM)-the MBL phase in one dimension at strong disorder. It yields an explicit and quantitative picture of the spatial boundary between localized and ergodic systems. We provide numerical evidence for this picture. When the theory is taken to its extreme logical consequences, it predicts that the MBL phase is destabilised in the long time limit whenever (1) interactions decay slower than exponentially in d = 1 and (2) always in d > 1. Finer numerics is required to assess these predictions.

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I. INTRODUCTION

The contrast between localized and thermalizing (ergodic) many-body systems is an exciting theme in condensed matter, touching upon foundations of thermodynamics. The topic goes back to the seminal work [1] but there has been revival due to some theoretical advances [2-5], powerful numerics [6-8], and the exciting experimental possibilities with cold atoms [9,10]. Most authors define many-body localization (MBL) as a property of the eigenfunctions at finite energy density: there is a full set of local conserved quantities-LIOM's "local integrals of motion" [11-13]. We start from this definition even if it is surely not literally applicable to all systems that have been labeled as MBL (e.g., systems with a mobility edge, including in particular systems with no quenched disorder) and definitely not to all systems that exhibit MBL-like dynamical features [14], e.g., classical disordered oscillator chains [15–17].

This means in practice that our discussion is about strongly disordered lattice quantum systems. We ask whether and how the localization in these strongly disordered systems is stable when we couple them to zero-dimensional, ergodic grains that are large but finite, in particular much smaller than the localized system. Such a setup occurs naturally in disordered systems where the ergodic grains arise from regions with anomalously weak disorder, see Fig. 1.

The Hamiltonian of an ergodic system (or, simply, a bath) is essentially described by random matrix theory (RMT) through the eigenstate thermalization hypothesis (ETH) [18,19]. Realspace renormalization theories for MBL and ergodic inclusions have been formulated [20–22] but they are rather mesoscopic than microscopic and not formulated in the language of RMT. This is at first sight logical since RMT is intrinsically connected with chaos and ergodicity. Nevertheless, we point out that a simple RMT theory is able to describe the breakdown of thermalization towards MBL in 1D. In this point of view, localization emerges as an instability of RMT.

The motivation for our theory grew out of the bizarre observation that is by now well-known to many people in the field of MBL: the "avalanche" or "Ice-9" [23] scenario. If a bath is coupled to a spin weakly, but strong enough to thermalize that spin, then the combined spin + bath system becomes ergodic and one is inclined to describe it simply by a random matrix. Doing so, the composed system looks like the original bath, except that its Hilbert space dimension is doubled and its level spacing is (roughly) halved. Therefore it is now an even more powerful bath. Iterating this argument blindly one is led to conclude that any localization must be destroyed by a large enough ergodic grain that can serve as the original bath! Obviously, we do not believe this scenario to be correct as it would rule out localization in strongly disordered 1d spin systems, where it has been almost proven [12]. The RMT used in the present paper is subtle enough to avoid this fallacy by tracking the evolution of the structure factors (spectral functions) of the added spins. The narrowing of these structure factor eventually brings the avalanche to a halt in 1d systems. More generally, our theory is able to describe correctly the stability of strong localization to ergodic grains in all cases where we know the answer: d = 1 interacting systems, and noninteracting systems.

Yet, the most striking prediction of the RMT theory developed in the present paper is that the avalanche scenario has a core of truth: any degrees of freedom that are added to a bath and that do get effectively thermalized by the bath, also fully contribute to that bath. By this we essentially mean that it is the level spacing of the joint system, which is hence smaller than that of the bath alone, that determines whether other weakly coupled degrees of freedom get thermalized or not. This leads to a simple, universal theory of thermalization, where the bath is characterized by a single dimensionless parameter G that is essentially defined as *matrix element level* spacing. This should be contrasted with the question about timescales of thermalization or transport [24,25], which is more complicated.

As a consequence, our RMT theory describes explicitly the spatial interface between an ergodic and a MBL system. In our theory, the crossover region is fully thermal, but the structure (spectral) factors of operators supported in that region become very narrow as their support approaches the MBL system.

An intruiging prediction of our theory is that a localized system with interactions that decay slower than exponentially

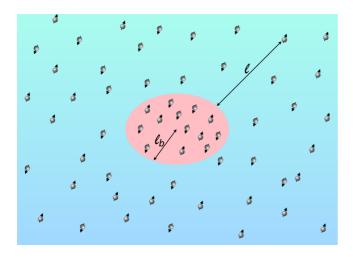


FIG. 1. The spins in the red region are closer to each other than in the surrounding blue-green region, hence they interact stronger. This stronger interaction leads to an "ergodic grain" in the red region. What is the effect of this grain on its localized environment?

with distance, is not stable with respect to large ergodic grains, though the thermalization time for such a system can still be enormously large, thus making it localized for all practical purposes. Counterintuitive as it might be, the idea that a few degrees of freedom can delocalize a much larger number of localized degrees of freedom, has by now been put forward already by several authors [26–29]. Numerics for larger systems is however needed to nail down this instability. Also higher-dimensional localized systems would be unstable within our theory.

Outline

In Sec. II, we develop our random matrix theory for coupling spins to a bath. Then, in Sec. III, this theory is applied iteratively to the ergodic grains coupled to localized material. Section IV focuses on the interface region between ergodic grain and localized material. We gather our numerical results and checks in Sec. V. The appendices contain technical issues that can be skipped in a first reading.

II. BATH+SPIN PROBLEM

Our method is to consider an ergodic system, that we call "bath", coupled locally to small systems, 1/2-spins for concreteness. As such, our setup is very familiar from open quantum systems, see, e.g., [30–33] for specifics of baths coupled to localized systems.

The point is, however, that we ask for detailed information on the eigenstates of the joint system, which will then be used to regard the joint system as a bath itself. For the sake of simplicity, we assume that energy is the only locally conserved quantity. We write the Hamiltonian as

$$H = H_S + H_B + H_{SB}$$

acting on $\mathcal{H}_B \otimes \mathcal{H}_S$ ("bath" \otimes "spin"), and, as conventional, we slightly abuse notation by writing $H_S = 1 \otimes H_S$, $H_B =$

 $H_B \otimes 1$, etc. To fix thoughts, we choose

$$H_S = h\sigma_S^z, \qquad H_{SB} = gV \otimes \sigma_S^z$$

with *V* a local operator acting in the bath (e.g., a σ^x operator on the site adjacent to the spin *S*), a coupling strength *g* and field *h*. We denote the eigenbasis of H_S by $|s\rangle$. Additional interaction terms such as $g'V' \otimes \sigma_S^z$ can be considered as well and do not introduce as such any substantial new difficulty; see Secs. III A and III D.

A. Properties of the bath: ETH

Let us denote in general by $|b\rangle$, E(b) the eigenvectors and energies of the bath Hamiltonian H_B . The important properties of the bath concern the matrix elements $V_{b,b'} = \langle b|V|b'\rangle$ in the *b* basis. We assume the ETH in the following form:

$$V_{b,b'} = \frac{1}{\sqrt{\rho}} \sqrt{v(\omega)} \eta_{b,b'}, \qquad b \neq b'.$$
(1)

Here, $\eta_{b,b'}$ are random variables of mean zero and unit variance, ρ is the density of states at maximum entropy (see later), and $v(\omega)$ is a positive function of $\omega = E(b) - E(b')$ with units of 1/energy, smooth on the scale of the level spacing. The dependence on the energy E = (E(b) + E(b'))/2 is less relevant since we naturally assume that v depends smoothly on the *energy density* $\varepsilon = E/N$, hence we omit it from the notation. The ETH also provides information on the diagonal elements, namely,

$$V_{b,b} = \langle b|V|b\rangle = \langle V\rangle_{\varepsilon}, \quad \langle b|VV^*|b\rangle = \langle VV^*\rangle_{\varepsilon}, \quad (2)$$

where $\langle \cdot \rangle_{\varepsilon}$ indicates the thermal ensemble at energy density $\varepsilon = E(b)/N$. By subtracting constants, we can simplify and set $\langle V \rangle_{\varepsilon} = 0$ at the relevant energy density. By (2), we have the following relation between the introduced quantities:

$$\sum_{b'} |V_{b,b'}|^2 = \langle VV^* \rangle_{\varepsilon}.$$

If, as we primarily have in mind, V is of the simple form $V = \sigma_B^x$, then $\langle VV^* \rangle_{\varepsilon} = 1$ if ε is at maximum entropy, as we will anyhow assume below. Using that v varies on a scale much larger than the level spacing and that the density of states is constant (see below), we can also write

$$\langle VV^* \rangle_{\varepsilon} = \int \mathrm{d}\omega v(\omega),$$
 (3)

and likewise, we can identify $v(\omega)$ with the dynamic structure factor at zero momentum:

$$\langle V(t)V^*\rangle_{\varepsilon} = \int \mathrm{d}\omega \, v(\omega) \mathrm{e}^{\mathrm{i}\omega t}$$

for t small enough so that single levels are not resolved, i.e., $\rho t \ll 1$, since we have assumed v to be smooth. Treating $\rho = \rho(E)$ as a constant is in general not a valid approximation as $\rho(E) \propto e^{s(\varepsilon)N}$ where the entropy density $s(\varepsilon)$ varies smoothly with ε . Hence

$$\ln(\rho(E + \Delta E)/\rho(E)) = s'(\varepsilon)\Delta E + s''(\varepsilon)(\Delta E)^2/N,$$

the primes referring to derivatives with respect to (w.r.t.) ε . From this, we see that at maximum entropy, i.e., $s'(\varepsilon) = 0$, we can yet treat $\rho(E)$ as a constant. Generalizing our arguments to other values of the energy density is straightforward, and it brings no new insight, therefore we stick to the above setting.

For baths with a local structure, the function v decays rapidly at large ω [34]; $v(\omega) \leq Ce^{-|\omega|/\xi}$ can be proven rigorously [35] with ξ of the order of the total energy per site. The behavior at small $\omega \leq \xi$ reflects the long-time transport properties, i.e., $v(\omega) \sim \omega^{d/2-1}$ for a diffusive system and $v(\omega) = \text{const.}$ below the Thouless energy, see [36–38] for details. For our purposes, these features are not important and for the moment, it suffices to think of v as a simple bump function with halfwidth ξ .

B. Basic RMT hypothesis

Our basic hypothesis describes the eigenstates of *H* based on three basic principles: (1) hybridization condition (matrix element \gg level spacing), (2) energy conservation, and (3) RMT is assumed whenever compatible with (1) and (2). Let us make this more precise. The energy difference between the 2 spin states $s = \pm 1$ is 2*h*, so the relevant matrix element of the perturbation is of size $g\sqrt{v(2h)/\rho}$, by (1), whereas the level spacing between states with opposite spin *s* is $1/\rho$. Hence the condition for hybridization is

$$\mathcal{G} \equiv g \sqrt{v(2h)\rho} \gg 1. \tag{4}$$

If the hybridization condition is not satisfied, then the spin is not thermalized by the bath and the coupled eigenstates are determined by perturbation theory. If the hybridization condition *is* satisfied then we propose a form for the new eigenstates, namely,

$$\psi = \frac{1}{\sqrt{2\rho}} \sum_{b,s} \sqrt{k(\omega)} \,\eta(s,b) \,|s,b\rangle, \quad \omega = E(s,b) - E.$$

As before, the $\eta(s,b)$ are independent and identically distributed (i.i.d.) random variables with zero mean and unit variance. E(s,b) = hs + E(b) is the energy of the eigenstate $|s,b\rangle = |s\rangle|b\rangle$ with respect to the uncoupled Hamiltonian $H_{S} + H_{B}$. The hybridization function $k \ge 0$ is assumed to be smooth on the scale of the level spacing $1/\rho$. It satisfies the normalization $\int d\omega k(\omega) = 1$, ensuring that $||\psi|| = 1$, and it has dimension energy⁻¹. The factor 2ρ is the density of states of the B + S system (recall ρ is the density of the bath). This ansatz expresses that the new eigenstates are random superpositions of uncoupled eigenstates, up to energy conservation which is expressed by the fact that the function k is cutoff at large $|\omega| \ge w$, where we have defined a *halfwidth* w. It is natural to assume that for $|\omega| \leq w$, the function k is essentially flat. In the next section, we refine the information on the function k, but for most of our applications such detailed information is not necessary: all that really matters is that wdoes not depend on the total Hilbert space dimension (or, equivalently, not on ρ).

C. The hybridization function k

Let us start by describing some general features of the hybridization function k. For $|\omega| \ge \xi$, it is easy to argue that k inherits the exponential decay of v. For some applications of our theory (see Sec. III D), we will also need to know the shape of k for intermediate $w \ll |\omega| \ll \xi$. Simple reasoning

based on perturbation theory (see also Sec. II E) yields that $k(\omega) \sim \omega^{-2}$, and it is therefore natural to propose for k a Lorentz shape

$$k(\omega) = \frac{1}{\pi w(1 + (\omega/w)^2)}$$

(obviously the exponential faloff $e^{-|\omega|/\xi}$ should be incorporated but this is not essential for our applications). Numerical tests, see Appendix A, confirm the asymptotic $k(\omega) \sim \omega^{-2}$. Figure 7 shows the hybridization curve for a real bath; we see that this curve has some structure for $|\omega| \leq w$, so the Lorentzian form is merely an idealization.

It remains thus to explain how to compute the halfwidth w. What rule to apply turns out to depend on the value of the inverse correlation time in the bath at the frequency 2h, i.e., on the characteristic ω_0 over which v changes appreciably around $\omega = 2h$. We distinguishes two cases: *Fermi's "golden rule"* (*FGR*). The FGR implies $w = g^2v(2h)$ provided that the rate w is smaller than the inverse correlation time in the bath ω_0 . In this paper, the FGR will be applicable most of the time, at least when taking into account a caveat that we postpone to Sec. II E. Note that as long as ξ is not smaller than 2h, the approximation $v(2h) \approx 1/\xi$ is reasonable and we have hence simply $w \approx g^2/\xi$. See Appendix A for numerical confirmation of the FGR expression for the width w.

Quasiadiabatic regime. One cannot apply consistently the FGR if the predicted hybridization width w becomes larger than ω_0 . However, the situations where the FGR does not apply play only a secondary role in our theory, and the discussion below can be skipped in a first reading (in particular, in the next paragraphs of this section, we will always assume that FGR holds whenever needed).

Breakdown of the FGR arises if v has a very sharp peak around $\omega = 2h$, i.e., if $w = g^2 v(2h) \gtrsim \omega_0$ (where w is the 'erroneous' width given by the FGR); since ω_0 is given by 1/v(2h) on the top of the peak, this reads also $v(2h) \gtrsim 1/g$. For us, a situation where the FGR does not apply will most prominently show up through interaction terms of the type $\sigma_i^z \sigma_j^z$ (for *i* and *j* nearest neighboring sites), see Sec. III A. This can also happen with a σ_i^x operator, though it results then from a very sharp resonance between near spins, see Sec. III D. To avoid changing setup, let us, however, stick to this case here, and let us assume that $g \gg \omega_0$. It is convenient to model the action of the bath on the external spin by a time-dependent Hamiltonian, i.e., to assume that the evolution of the spin is governed by the Hamiltonian

$$H_S(t) = g \cos(2ht)\varphi(t)\sigma_S^x + h\sigma_S^z$$

where φ is a (stochastic) function of time such that the time correlation $\langle \varphi(t)\varphi(0) \rangle$ decays as $e^{-\omega_0 t}$. For the intermediate time scales $\omega_0 t \ll 1$, the dynamics is dominated by the oscillatory factor $\cos(2ht)$, and it is convenient to move to the rotating frame to get rid of this oscillation (since the external frequency is exactly tuned with the energy gap of the spin, the rotating frame is nearly given by the vectors $|\alpha_{\pm}\rangle = e^{i2ht}|\uparrow\rangle \pm e^{-i2ht}|\downarrow\rangle$). In this basis, one may now compute the rate at which the dynamics flips $|\alpha_{\pm}\rangle$ to $|\alpha_{\mp}\rangle$. Since the evolution of the system is quasiadiabatic, and that the Hamiltonian evolves at rate ω_0 , one expects flips to also occur at rate ω_0 , see Ref. [39]. Hence in this case, one gets also for the hybridization width $w = \omega_0$.

D. New structure factor

Let us determine the matrix elements of a bath operator V upon adding the spin when the new eigenfunctions are as described in the previous section via a hybridization function k. This is a straightforward calculation starting from

$$V_{\psi,\psi'} = \sum_{s,b,b'} \langle \psi | b, s \rangle V_{b,b'} \langle b', s | \psi' \rangle, \tag{5}$$

where we used that V acts on the bath only and ψ, ψ' are eigenfunctions (at energies E, E') of the coupled system. We use that V had a vanishing diagonal in the b basis and, at least at maximal entropy, this remains so in the new basis [40]. For the off-diagonal, we replace $V_{b,b'}, \langle \psi | b, s \rangle, \langle b', s | \psi' \rangle$ by their explicit (random) expressions. Pretending that all random variables are independent, we get that the variance of $V_{\psi,\psi'}$ is given by

$$\langle |V_{\psi,\psi'}|^2 \rangle = 2 \frac{1}{4\rho} \int d\omega_1 d\omega_2 \, k(\omega_1) k(\omega_2) v(\omega - \omega_1 - \omega_2),$$

where $\omega = E - E'$ and the factor 2 in front originates from the sum over the spin variable *s*. Making again an independence assumption, we conclude that the new system satisfies again ETH in the sense of (1) with density $\rho' = 2\rho$ and structure factor

$$v'(\omega) = (k \star v \star k)(\omega), \tag{6}$$

where $(a \star b)(\omega) \equiv \int d\omega_1 a(\omega_1) b(\omega - \omega_1)$ is a convolution of functions.

The upshot is that the function v' is given by v smoothened twice with halfwidth w. In particular, if $g^2/\xi \ll \xi$, which is the case we have in mind, then the two functions v' and vare nearly the same. Of course, as the density of states ρ is doubled, this means that the typical matrix element of Vdid become smaller by a factor $\sqrt{2}$. On the one hand, this is a very intuitive conclusion: the new spin has made the bath more powerful by increasing its effective dimension. On the other hand, the conclusion that the structure factor of a bath operator is unaffected by the coupled spin that is potentially much slower than the bath correlation time, does not hold up to scrutiny [41]. Indeed, the correlation function $\langle V(t)V \rangle_{\varepsilon}$ should acquire long lived oscillations with frequency $\omega = \pm 2h$ due to the slow spin. Below, in Sec. IIE, we explain how this feature emerges within our formalism upon refining the RMT assumption. Since this does not affect our results, we however ignore this in the rest of the paper.

Finally, let us now also determine the structure factor of an operator on the coupled spin, $V = \sigma_S^x$, i.e., $\langle b, s | V | b', s' \rangle = \delta_{b,b'} \delta_{s,-s'}$. Instead of (5), we start now from

$$V_{\psi,\psi'} = \sum_{s,b} \langle \psi | b, s \rangle \langle b, -s | \psi' \rangle \tag{7}$$

Using analogous steps as the derivation of (6), we find for the new structure factor

$$v'(\omega) = \frac{1}{2}(k \star k)(\omega + 2h) + \frac{1}{2}(k \star k)(\omega - 2h).$$
 (8)

This represents two bumps centered at $\pm 2h$ of halfwidth 2w. Note that $\int v' = 1$ (since $\int k = 1$), which is consistent with $\int v' = \langle VV^* \rangle_{\varepsilon}$, see (3). The expression (8) can simply be obtained from (6) by putting $v(\omega) = \frac{1}{2}\delta(\omega + 2h) + \frac{1}{2}\delta(\omega - 2h)$, which can indeed be considered as the structure factor of σ_S^x with respect to the uncoupled Hamiltonian $H_S + H_B$.

E. Backreaction correction

As already remarked above, our theory misses a backreaction effect that creates spikes in the bath structure factor. We investigate now a refinement of the theory that does allow to recover those spikes.

We write in general $H_0 = H_S + H_B$ and the corresponding energies as E(b,s). We choose a target energy E and we let P be the spectral projection associated to H_0 of the interval [E - w, E + w] with some halfwidth w that we will assume to be the same as the halfwidth introduced above, even though this is not necessary for the upcoming lemma. Also, we write $\overline{P} = 1 - P$. Our main tool is the following simple principle, whose proof follows directly from the eigenvalue equation.

Lemma 1. Schur complement formula. Let ψ be an eigenvector of H with eigenvalue E and $P\psi \neq 0, \bar{P}\psi \neq 0$, then $\bar{P}(E - H)\bar{P}$ is invertible on $\bar{P}H_{SB}P\psi$ and

$$\bar{P}\psi = \frac{1}{\bar{P}(E-H)\bar{P}}\bar{P}H_{SB}P\psi.$$
(9)

This formula expresses a useful structural relation between the spectral regions close to and far from the energy E.

An obvious way to take this relation into account is to retain the random matrix form of the eigenstates ψ inside the interval [E - w, E + w], i.e., for $P\psi$, but to relate $\bar{P}\psi$, i.e., outside the interval [E - w, E + w], to $P\psi$ by the above Lemma II E. This means that we no longer assume that all $\eta(b,s)$ in Sec. II B are independent, but just those inside the interval [E - w, E + w]. Hence we write $\psi = P\psi + \bar{P}\psi$ and we postulate

$$P\psi := \frac{1}{\sqrt{2\rho}} \sum_{b,s} \sqrt{k_0(\omega)} \eta(b,s) |b,s\rangle, \tag{10}$$

where again $\omega = E - E(b,s)$, $\eta(b,s)$ are independent random variables with mean zero and unit variance, and we have introduced a cutoff hybridization function $k_0(\omega) := \chi(|\omega| \le w)k(\omega)$. The remainder $\bar{P}\psi$ is then obtained by (9). This model for ψ refines the proposal in Sec. II B. Within this model, let us now calculate $v'(\omega)$, the updated structure factor of σ_B^x , i.e., we refine the result of Sec. II D. We start from the decomposition

$$\langle \psi | \sigma_B^x | \psi' \rangle = \langle P \psi | \sigma_B^x | P' \psi' \rangle + \langle P \psi | \sigma_B^x | \bar{P}' \psi' \rangle + \langle \bar{P} \psi | \sigma_B^x | P' \psi' \rangle + \langle \bar{P} \psi | \sigma_B^x | \bar{P}' \psi' \rangle.$$
(11)

Here the primed projectors $P', \bar{P}' = 1 - P'$ are associated to ψ' ; i.e., they are centered on E' instead of E. The new effect can be seen most easily on the second (or third) term. Using Lemma II E and plugging $H_{SB} = g\sigma_S^{x}\sigma_B^{x}$, we get

$$\langle P\psi|\sigma_B^x|\bar{P}'\psi'\rangle = \sum_{b,b',s,s'} \langle P\psi|b,s\rangle K(b,s|b',s')\langle b',s'|P'\psi'\rangle$$
(12)

with the first and last factors given still by the RMT ansatz and

$$K(b,s|b',s') = g\langle b,s|\sigma_B^x \frac{1}{\bar{P}'(E'-H)\bar{P}'}\bar{P}'\sigma_S^x\sigma_B^x|b',s'\rangle$$

Whereas we know that the diagonals $\langle \psi | \sigma_B^x | \psi \rangle$ vanish (see Sec. II D), there is in general no reason why K(b,s|b',s')should vanish for b = b'. These partially diagonal terms yield contributions to the structure factor v' that are not directly related to v but are instead peaks of halfwidth 2w around $\omega = 0$ and $\omega = \pm 2h$. To be specific, up to the lowest nonvanishing order in g, we find, see Appendix B, the following contribution to v':

$$\mathcal{W} k_0 \star \delta(\cdot \pm 2h) \star k_0, \quad \mathcal{W} \equiv \left(\frac{g}{\max \xi, |h|}\right)^2,$$
(13)

i.e., two peaks with weight W and halfwidth 2w, from the smoothing with k_0 (the fact that we get here k_0 instead of k is most likely irrelevant). These peaks are located at the Bohr frequencies of the external spin $\pm 2h$, fully in line with the intuition from the time-domain.

The contributions from $K(\cdot)$ with $b \neq b'$, together with the first term in (11), basically recreate the previously found form of $v'(\omega)$, up to normalization (see below). In fact, the calculations coming here can also be used to justify the choice of the width, i.e., the FGR, see Appendix B.

Putting all pieces together, we find within our refined model, and up to lowest nontrivial order in g, that the structure factor v' is given by

$$(1 - 2\mathcal{W})k \star v \star k + \mathcal{W}k_0 \star \delta(\cdot \pm 2h) \star k_0.$$
(14)

The factor (1 - 2W) is due to the overall normalization $\int v' = 1$. In the relevant case $w \ll \xi$, the new peaks are less smooth than the structure factor of the original bath, but then $W \ll 1$. Hence then the strength of the smooth part of the bath has been slightly depleted by the appearance of narrow peaks.

Let us discuss the implications of the refinement presented above as we will apply the theory iteratively, in Sec. III. First, as we will now be dealing with a situation where the structure factor v is a sum of a smooth part $v_{\rm sm}$ and a more irregular part with narrow spikes $v_{\rm irr}$, with $\int v_{\rm irr} \ll \int v_{\rm sm}$, we have to reconsider the reasoning in Sec. II C on the hybridization width. In such a case, it can happen that the Fermi's "golden rule" is applicable for $v_{\rm sm}$ but not for v itself and then we have $w \approx g^2 v_{\rm sm}(2h)$ (a superficial justification of this is given in Appendix B).

Secondly, since we will couple spins with rapidly decaying couplings g_i to the same bath, we will get a depletion of the smooth structure factor by the factor $\prod_i (1 - 2W_i)$ with $W_i \equiv (\frac{g_i}{\max(\xi, |h_i|)})^2$. Because of the rapid decrease of g_i , this factor will still be close to 1 and so the overall depletion effect remains small. Hence the conclusion is that the refinement proposed in this section, does not have any implications for us, and we will henceforth ignore it.

F. Limitations of our theory

Our theory makes some uncontrolled assumptions. In particular, apart from the refinement introduced in Sec. II E [42], we assume that the matrix elements of a bath operator V as well as the parameters $\eta(b,s)$ featuring in the hybridization

function are all mutually independent. This assumption is definitely the main source of nonrigor.

Locality. In effect, our theory provides an expression for the eigenstates of the coupled system as a random superposition of the states of the uncoupled system, taking into account conservation laws. Upon iterating, these putative eigenstates are random superpositions of products over sites. This picture can never fully capture locality. The same problem occurs if one would use the Berry conjecture [43] (eigenstates are random superpositions of plane waves with appropriate momenta) as a cartoon for ETH in many-body systems. The rapid decay of the structure factor $v(\omega)$ as $\omega \to \infty$ is not captured by this cartoon and it needs to be imposed explicitly. Also our theory sometimes misses the decay of structure factors: If we build up an ergodic chain of lenght ℓ by coupling spins with $g \sim h \sim \xi$, then our theory predicts that each coupled spin broadens by a similar amount the structure factors and eventually some local operators have a width of order ℓ , analogously to a featureless random matrix with the same bandwidth. More generally, this issue leads to a clear error if the total broadening is comparable or larger than the original width ξ of bath operators, which occurs, roughly speaking, if $\sum_i g_i^2 \ge \xi^2$ with g_i the coupling strengths of added spins.

For our purposes, we can largely circumvent this issue. The first reason for this is that, resorting to the LIOM representation for the localized part of the system, we can encode most of the locality through the exponential decay in space of the coupling of LIOMs to the bath. Obviously the problem of encoding the locality inside the bath and its close vicinity remains unresolved in that way, but this is of little practical relevance since the size of baths that we will consider (i.e., ergodic spots in an otherwise localized material) are very small as compared to the distance among them.

The second, somehow deeper, reason is that we can actually devise a careful way to apply our theory so as to avoid inconsistent results. Indeed, in d = 1, we will actually manage to exhibit locality without using the representation by LIOMs in the localized phase (see Sec. III D) so that the first reason does not apply. As we will see there, it is actually still possible to correctly encode the locality of a single spin coupled to a bath, i.e., we get a realistic frequency decay for the structure factor of this spin. The problem only comes if we we first couple many spins one be one, then represent the eigenstates as a superposition of product states, and finally try to recover the locality properties of a spin incorporated at the beginning of the procedure. As argued above, this is bound to fail. However, in the cases that we had to deal with, this problem just didn't show up, since we never had to evaluate the structure factor of a spin after that other spins have been coupled to the system.

Proximity effects. These are effects [44,45] whereby a localized system localizes the bath by inducing effective disorder terms via the coupling. These effects arise when the coupling to the localized system dominates the ergodic bath Hamiltonian. If we keep coupling spins with coupling strenghts g_i directly to a finite bath, then proximity effects will occur when $(\sum_i g_i^2)^{1/2}$ becomes comparable to the total bath energy but our theory is unable to detect this. This scenario is however not realized in the systems studied in this paper.

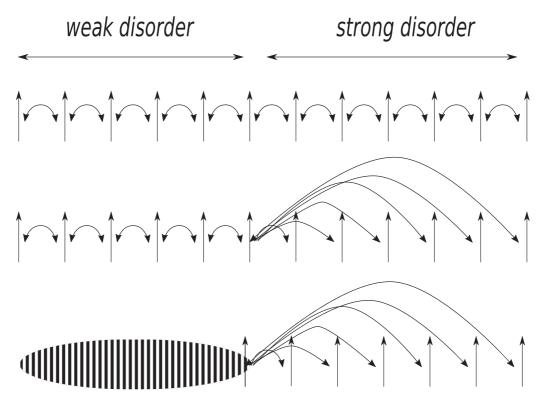


FIG. 2. (Top) A chain of weakly disordered spins—the ergodic grain—is coupled to a chain of strongly disordered spins—the MBL system. (Middle) The system is modelled by weakly disordered spins coupled to LIOMs (no coupling between the LIOMs any more). Note that all LIOM's are coupled only to the rightmost spin. (Bottom) The weakly disordered spins are sometimes modeled by a random matrix.

III. STABILITY AGAINST ERGODIC GRAINS

A. Stability of one-dimensional localization

We apply our theory to a bath of ℓ_b spins attached to a strongly localized spin chain of length ℓ at its right. However, instead of considering ℓ weakly coupled disordered spins, we invoke the LIOM theory and we consider ℓ uncoupled l spins. The *l*-spin operators are denoted by $\tau_i^{x,y,z}$ instead of $\sigma_i^{x,y,z}$, and the τ_i^z commute with the Hamiltonian of the ℓ -stretch. This Hamiltonian does hence not contain any more terms that flip the τ^z .

The LIOMs are exponentially localized in the following sense. One can expand the quasilocal operators τ_i (we omit the superscripts x, y, z since they play no role here) in strictly local operators as $\tau_i = \sum_{I \ni i} \tau_{i,I}$, where *I* are lattice intervals, i.e., sets of consecutive points on the lattice, containing *i*. In the localized phase, these operators decay exponentially in norm for typical realizations of the disorder. We define the localization length (in lattice units) as

$$\frac{1}{\zeta} = \lim_{|I| \to \infty} \frac{1}{|I|} \left(\ln \frac{1}{\|\tau_{i,I}\|} \right), \tag{15}$$

where |I| is the number of lattice sites in the interval I, and where $\langle \cdot \rangle$ denotes the average over the disorder.

When a bath of ℓ_b spins is coupled to the localized systems of ℓ localized spins, the strictly local coupling of the leftmost of the ℓ spins to the bath, gives rise to a nonlocal, though exponentially decaying, coupling of the *l* spins to the bath, see Fig. 2. This setup is captured by the Hamiltonian

$$H = H_B + \sum_{i=1}^{\ell} h_i \tau_i^z + \sum_{i=1}^{\ell} g_i \sigma_0^x \otimes \tau_i^x,$$
(16)

with decaying couplings

$$g_i = g_1 e^{-(i-1)/\zeta}$$

Note that all the *l* spins are coupled to the same bath operator σ_0^x and that g_1 is the coupling strength of the leftmost physical spin to the bath.

The following kind of terms were suppressed in our model Hamiltonian (16): (1) nonlocal LIOM-energy terms like, e.g., $\tau_i^z \tau_{i+1}^z$, and (2) bath couplings affecting multiple LIOMs like $\sigma_0^x \otimes \tau_1^x \dots \tau_i^x$. These terms are indeed generically present in genuinely interacting systems. Nevertheless, we prefer to first ignore them and to study the Hamiltonian (16) taken literally, so as to focus on the main point of our argument. Let us stress that, even so, the Hamiltonian as defined by (16) is neither free nor integrable, since the bath Hamiltonian H_B is assumed to obey ETH, so that the full system remains interacting through the influence of the bath. In a second step, we briefly indicate how to incorporate additional interaction terms.

Localization for the Hamiltonian (16). We take $h_i \sim \xi$ with ξ the halfwidth of the structure factor v of the bath operator σ_0^x . This is realistic if the bath is made up from similar spins as the localized chain. Of course, the h_i should be disordered but this is not important any longer in (16): the strong disorder has already been used to derive this model Hamiltonian, and

it is reflected in $g_1 \ll \xi$ and $\zeta \ll 1$. In particular, we may use the FGR to compute the hybridization width.

We proceed inductively, setting first $g_i = 0$ for i > 1. That puts us precisely in the case discussed at length in Section II, with $V = \sigma_0^x$. The hybrdization condition (4) will be clearly satisfied if ℓ_b is large enough and we obtain eigenstates ψ of the $B + S_1$ system. The next step is to view the $B + S_1$ system as a the bath and to couple it to S_2 through $V = \sigma_0^x$. If ℓ_b is large enough, the hybridization condition is again satisfied and we can proceed. The only way that our scheme can stop is if at some point the hybridization condition is violated. To evaluate the hybrdization condition we need to determine at each step the new density of states ρ' and structure factor v' from those at the previous step ρ , v. Naturally, $\rho' = 2\rho$ and from (6) in Sec. II D we deduce that, roughly, $v' \approx v$: the structure factor stays roughly the same since the sum of widths of all the hybridization functions is small compared to the width of v: $\sum_{i} g_{i}^{2} / \xi \ll \xi$. This means that the \mathcal{G} parameter defined in (4) gets updated as

$$\mathcal{G}' = \mathcal{G}e^{-a}, \quad a \equiv 1/\zeta - \ln(2)/2 \gg 0,$$

where the inequality $a \gg 0$ follows from strong disorder $\zeta \ll 1$. It follows that $\mathcal{G}_{\ell} = e^{-a\ell}\mathcal{G}_1$. Since $\mathcal{G} \approx (g_0/\xi)2^{\ell_b/2}$, by ETH for the original bath, we conclude that the hybridization condition breaks down at $\ell = \ell_c$ with

$$\ell_c \approx \frac{\ln 2}{2/\zeta - \ln 2} \ell_b \tag{17}$$

and this length is hence an estimate for the size of the crossover region. In a more general estimate, the factor ln 2 should of course be replaced by an entropy density.

Note that our estimate differs from the more simple guess whereby one considers only the thermalizing effect of the original bath with length ℓ_b ; such an estimate leads to a crossover region of size

$$\ell_c \approx \zeta \frac{\ln 2}{2} \ell_b.$$

More importantly, our estimate implies that LIOM's can not have an arbitrarily large localization length, as defined by Eq. (15), because if $2/\zeta \leq \ln 2$, then the localization is not stable with respect to ergodic grains.

Additional interaction terms. Let us briefly discuss what happens in the presence of additional terms in the Hamiltonian (16). When dealing with the $i^{\text{th}} l$ spin, we have a Hamiltonian of the form

$$V_h^x \otimes \tau_i^x + V_h^z \otimes \tau_i^z$$
.

Besides the coupling $\sigma_0^x \otimes \tau_i^x$ that we dealt with already, the term $V_b^x \otimes \tau_i^x$ includes terms of the form $\sigma_0^x \otimes \tau_1^x \dots \tau_i^x$. The term V_b^z comes from the interaction terms among l spins, i.e., $\tau_{i-1}^z \tau_i^z$, and more generally $\tau_1^x \dots \tau_i^z$. The consideration of these terms mainly induces the two following modifications: (a) Breakdown of the FGR. Let us deal with the term $V_b^z \otimes \tau_i^z$ alone, and let us imagine that it is simply given by $\tau_{i-1}^z \tau_i^z$. This operator does not flip the l spin at i, hence the eigenstates are now of the form $|b_\uparrow,\uparrow\rangle$ or $|b_\downarrow,\downarrow\rangle$, where \uparrow and \downarrow represent the state of the l spin at i. The operator τ_{i-1}^z only hybridizes the states within the bath in a way that depends on the state of τ_i . However, far away from the original bath, the structure

factor of the operator τ_{i-1}^{z} will have a narrow peak at origin, because the $(i-1)^{\text{th}} l$ spin is so weakly coupled to the original bath. Hence the FGR will not apply, and one has instead to estimate the hybridization width by 1/v(0) as we argued in the second part of Sec. II C. This is in fact not an issue: one simply needs to apply the correct rule as to avoid an absurdly large hybridization width.

(b) Breakdown of the product structure. Let us now add the operator $V_b^x \otimes \tau_i^x$, on top of $V_b^z \otimes \tau_i^z$. The basis made of the states $|b_{\uparrow},\uparrow\rangle$ and $|b_{\downarrow},\downarrow\rangle$ does not enjoy the product structure anymore. This again is as such not an issue as the theory developed in the previous section did not actually rely on this. This said, when computing the structure factor of τ_i^x , one should keep in mind that there is no strict orthogonality relation among the states $|b_{\downarrow}\rangle$ and $|b_{\uparrow}\rangle$. Instead, one should use the narrow hybridization width obtained in (a) to recover a result in agreement with the upshot obtained for the Hamiltonian (16) without any extra terms.

B. Instability of MBL for subexponentially decaying interactions

The above analysis directly implies that a spin chain with subexponentially decaying interactions [46,47] is not stable wit respect to ergodic grains. Indeed, if such a system were MBL, then the LIOM operators should presumably have a subexponential tail as well [48] and we can model their interaction with an ergodic grain by taking the g_i in (16) to decay subexponentially. In this case, however, the \mathcal{G} parameter flows to infinity if ℓ_b is large enough, i.e., if the grain is sufficiently large. A first step towards verifying this is described in Sec. V, where we consider a random matrix corresponding to a 6-spin bath coupled weakly to a chain of 8 LIOM spins with decay factor $e^{-1/\zeta} = g_{i+1}/g_i = 3/4$, for which $\ell_c = \infty$ according to the above estimates (i.e., we do not even consider subexponentially decaying interactions but exponential ones with a too slow decay rate for localization to persist). Despite the LIOM chain being localized, we see that the resulting system indeed behaves rather accurately as an ergodic system with dimension 2^{6+8} .

Finally, note that if we would change the model, so as to have very slowly decaying g_i , then proximity effects, see Sec. II F, can indeed localize the ergodic grain. We do not discuss this as such models can probably not emerge as LIOM's of local localized Hamiltonian [49,50].

C. Instability of MBL for higher-dimensional systems

The higher-dimensional setup is in effect similar to the case of subexponentially decaying couplings. Consider a spherical ergodic grain of with radius ℓ_b , surrounded by LIOM's coupled to it with strength decaying exponentially in distance r, $g_r \approx g_0 e^{-r/\zeta}$. The nearby LIOM's will get thermalized and according to our theory above, any thermalized LIOM fully contributes to the bath. The number of LIOM's with distance $r \leqslant \ell$ is

$$N_{\ell} = C_d (\ell_b + \ell)^d - \ell_b^d$$

with C_d the volume of a unit *d*-dim sphere. When these LIOM's have been thermalized, the bath density of states has been

increased by a factor $2^{N_{\ell}}$, which grows superexponentially in ℓ if d > 1. This overwhelms hence the effect of exponentially decreasing couplings. Said a bit differently, if there were a crossover region extending up to a distance ℓ_c from the bath, and beyond that region MBL would persist, then there is a thermal volume (bath+crossover region) $V_{\text{th}}(\ell_c) = C_d(\ell_b + \ell_c)^d$. The condition that spins outside the ergodic region are not hybridized is then

$$V_{\rm th}(\ell_c)\ln 2 - \frac{2}{\zeta}l_c \leqslant 0. \tag{18}$$

This equation has a finite solution for ℓ_c either when ℓ_b is small enough compared to ξ , or for d = 1 as soon as [51] $\xi < 1/\ln 2$.

Of course, this estimate is known already as an upper bound on the crossover region; it is, for example, the main reason why the analysis of [12], in which the crossover region is called "collar" is restricted to d = 1. The point in the present paper is however that within our theory, the volume V_{th} is not an upper bound, but the actual volume of a fully ergodic region.

As a note of caution, we remark that the d > 1 setup is not entirely free of the problem discussed in Sec. II F *locality*. Already when coupling the first layer of spins around a spherical ergodic grain of diameter ℓ_b , the structure factors in the grain grow like $\ell_b^{d/2}$ if we were to apply our theory literally.

Finally, we note that our conclusions echo the analysis in Ref. [30], where a careful investigations of structure factors led to a division of MBL systems in "weak" and "strong" MBL, where only d = 1 systems with exponentially decaying interactions can be "strong MBL". Our analysis suggests, however, that "weak MBL" systems are delocalized.

D. Stability of MBL without LIOM's

In this section, we rederive the stability of one-dimensional MBL that was established in Sec. III A. However, we do not use the powerful LIOM representation for the localized spins. Instead, we develop our reasoning here for physical spins instead of l spins. The possibility of doing so demonstrates the versatility of the theory.

Hence we consider again the Hamiltonian (16), but now written in terms of the physical σ operators:

$$H = H_B + \sum_{i=1}^{\ell} h_i \sigma_i^z + g \sum_{i=1}^{\ell} \sigma_{i-1}^x \otimes \sigma_i^x$$
(19)

with again σ_0^x a bath operator, cf. (16), and h_i random fields, i.i.d. random variables uniformly drawn from [-h,h] with $g/h \ll 1$, i.e., strong disorder. Let us denote by $v_i, i = 0, 1, ...$ the structure factor of the operator σ_i , these are relevant because they couple to spin i + 1. For v_0 , we take a bump function with halfwidth $\xi \sim h$ (as before), and the other v_i are to be determined. We write w_i for the width of the hybridization function by which the *i*'th spin is coupled to the preceding ones. So, assuming the FGR applies (see below) we have

$$w_i = g^2 v_{i-1}(2h_i). (20)$$

The structure factors v_i , $i \ge 1$ are given through (6) as

$$v_i(\omega) = \frac{1}{2\pi w_i} \left(\frac{1}{1 + \left(\frac{\omega + 2h_i}{2w_i}\right)^2} + \frac{1}{1 + \left(\frac{\omega - 2h_i}{2w_i}\right)^2} \right)$$
(21)

because the convolution of two Lorentz distributions with halfwidth w_i is again a Lorentz distribution with halfwidth $2w_i$. The above two relations (20) and (21) in determine inductively all structure functions. Let us neglect resonances by pretending that all neighboring fields are sufficiently different:

$$\min |h_i - h_{i-1}|, |h_i + h_{i-1}| \approx h/2.$$

Keeping then only the largest of two terms in (21) and using that $h/w_i \gg 1$, we get

$$w_i = g^2 v_{i-1}(2h_i) \approx \frac{g^2 w_{i-1}}{\pi h^2}.$$
 (22)

So the upshot is that the hybrdization width decreased by a factor of order $(g/h)^2$ (the calculation is not precise enough to take the prefactor π seriously). Iterating this and recalling that $w_0 = \xi$, we get

$$w_i = v_{i-1}(2h_i) = \xi(g/h)^{2i},$$

i.e., an exponentially decaying width for the structure factors. By comparison with III A, the decay rate $\ln(h/g)$ is a natural estimate for the inverse of the localization length ζ .

We recall that the whole iterative calculation makes sense only as long ETH is satisfied, hence as v is smooth on the scale of the level spacing. This means that this procedure breaks down when $w_i = 1/\rho_i$ where $\rho_i = 2^i \rho_0 \approx 2^{i+\ell_b}/\xi$, hence the breakdown is at $i = \ell_c$ with

$$2^{\ell_b} (2(g/h)^2)^{\ell_c} = 1,$$

which yields the same conclusion as (17) upon identifying $e^{-\zeta} = g/h$.

Let us now return to the validity of the FGR in this situation. The scale ω_0 over which v changes at ω can be estimated by $\omega_0 \approx \frac{v(\omega)}{|v'(\omega)|}$, so the FGR condition $w \ll \omega_0$ reads (for coupling the i + 1-th spin)

$$g^2 |v_i'(2h_{i+1})| \ll 1.$$

For i = 0, this means $g \ll \xi$, which was assumed, and for $i \ge 1$, it boils down to

$$\left(\frac{g}{w_i}\right)^2 \ll \frac{\left(1 + \mathcal{M}_i^2\right)^2}{\mathcal{M}_i}, \quad \mathcal{M}_i \equiv \frac{\min|2h_{i+1} \pm 2h_i|}{w_i}$$

which is indeed satisfied in the treatment above (except at resonances).

Finally, we notice that the Hamiltonian (19) does not contain any interaction terms such as $\sigma_i^z \sigma_{i+1}^z$, that are naturally present in one-dimensional systems to break their integrability, and it would be definitely desirable to deal with them as well. This can be done, at the cost of some modifications, that are basically the same as the one explained in the last part of Sec. III A. This said, we would like to stress the fact that it is here really crucial to take account of the fact that the FGR may not apply. Indeed, in order to proceed with our derivation, one must make sure that the width of the structure factors of a local operator at distance *i* from the bath decays as $e^{-i/\zeta}$. Contrary to

what happened for $\sigma_i^x \sigma_{i+1}^x$ couplings, the $\sigma_i^z \sigma_{i+1}^z$ will be "resonant", i.e., the structure factor of σ_i^z will have a peak at origin (once inserted into the bath) with width proportional to $e^{-i/\zeta}$, and, since the operator σ_{i+1}^z does not flip the spin, this peak will dominate the coupling. For this reason, the FGR does not apply. Instead the width of the resulting hybridization is proportional to the width of the peak, i.e., to $e^{-i/\zeta}$. Thus one concludes that the addition of the $\sigma_i^z \sigma_{i+1}^z$ will indeed not lead to a broadening of the structure factor and our derivation can proceed.

IV. STRUCTURE OF THE INTERFACE REGION

Let us discuss the most striking properties of the spatial interface region between an ergodic and an MBL system, referred to as the crossover region in Sec. III. First of all, our theory describes this interface region as fully thermal or ergodic: *ETH holds for all local operators in the crossover region*. However, the onset of localization is revealed by the narrowing of structure factors. Indeed, adopting the framework of Secs. III A and III B, the structure factor v_i of an operator located at the *i*'th added spin, has two main peaks of halfwidth w_i of the order

$$w_i \approx g_i^2 / \xi \approx e^{-2(i-1)/\zeta} g_1^2 / \xi$$

This follows from applying the formula (8) and it matches with the alternative derivation presented in Sec. III D. To avoid confusion, we stress that previously the symbol w was reserved for the (half)width of hybridization functions. Since the widths are exponentially decreasing, we see that adding further spins (i.e., i + 1, i + 2, ...) does not significantly affect the widths of the spins already added and so w_i above is the width regardless of how many more spins have been added.

To quantify the behavior in the interface region, we calculate an *inverse participation ratio* (IPR) of operators O in this region. By the IPR of O, we mean that we choose an eigenstate ψ (at maximal entropy, to stay within the setup) and we look at the distribution over the other eigenstates ψ' of the matrix elements

$$\langle \psi' | O | \psi \rangle.$$

The IPR(O) = IPR(O, ψ) is then

$$\operatorname{IPR}(O) = \left(\sum_{\psi'} |\langle \psi'|O|\psi\rangle|^4\right)^{-1}$$

(this quantity should be normalized by $\sum_{\psi'} |\langle \psi'| O | \psi \rangle|^2$ but we will always take $O = \sigma_i^{x,y,z}$ so that the normalization constant is always 1). Let us calculate this in terms of the parameters used in the ETH hypothesis, notably the structure factor v. Then

$$\mathrm{IPR}(O) = \rho \bigg(\int \mathrm{d} \omega v^2(\omega) \bigg)^{-1}.$$

If the structure factor v consists of two peaks with halfwidth w, then on its support $v \approx 1/(4w)$ and this yields

$$IPR(O) = 4\rho w$$

Note that hence $IPR(O) \approx \mathcal{N}$ where \mathcal{N} is the number of states or "effective dimension" within an energy range 4w, so this matches with the meaning of IPR in one-particle systems. As \mathcal{N} scales exponentially with system size, it is natural to consider rather the logarithm of IPR's, so we define

$$\mathcal{D}(O) = \ln \operatorname{IPR}(O).$$

Let us now apply this to the spins added to the bath, i.e., $O = \sigma_i^x$ for example. Let us assume that ℓ spins have been added to a bath of length ℓ_b and these spins have been thermalized, i.e. $\ell \leq \ell_c$ with ℓ_c as in (17). For the density of states ρ , we of course have to use the density due to all the spins, i.e., $\rho_\ell = 2^{\ell_b + \ell} / \xi$ (we neglect a volume denominator by pretending that ξ is the total bandwidth of the bath). This means that we have

$$\mathcal{D}(\sigma_{0}^{x}) = V_{\text{th}} \ln 2,$$

$$\mathcal{D}(\sigma_{i}^{x}) = \ln(4\rho_{\ell}w_{i}), \qquad i \ge 1,$$

$$\sim \ln(4\rho_{\ell}w_{1}) - 2(i-1)/\zeta$$

$$\sim \ln 4 + V_{\text{th}} \ln 2 - 2\ln\left(\frac{g_{1}}{\xi}\right) - 2(i-1)/\zeta, \quad (23)$$

where $V_{\text{th}} = l_b + \ell$ is simply the volume of the thermal region (original bath plus thermalized spins) and we used $w_1 = g_1^2/\xi$, and $\mathcal{D}(\sigma_0^x) = V_{\text{th}} \ln 2$ (the operator inside the bath).

It is worth spelling out the two aspects contained in (23), holding in fact for arbitrary operators O_i located around *i*. First, all the spins in the crossover region maximally participate to the effective dimension of the bath for an operator inside the ergodic grain, since $\mathcal{D}(O_{i=0})$ is proportional to V_{th} and not to ℓ_b . Second, $\mathcal{D}(O_i) - \mathcal{D}(O_1)$ decays linearly in *i* for operators inside the crossover region. Both of these aspects seem to be well-confirmed by the numerics in Sec. V.

More generally, for a subcritial grain [i.e., if (18) admits a solution for ℓ_c] in $d \ge 1$, we can consider also $\ell \ge \ell_c$. The theory predicts a smooth transition between the core of the grain and the MBL region. The MBL region is reached when $\mathcal{D}(O) \approx 0$, which of course reproduces the estimate (17) for ℓ_c in d = 1.

V. NUMERICAL TESTS

A. LIOMs coupled to a random matrix bath

In this section, we test the central prediction of our theory; that every spin, however weakly coupled, that is thermalized by the bath, indeed doubles the effective dimension of the bath. We consider again the Hamiltonian introduced in (16):

$$H = H_B + \sum_{i=1}^n \left(g_i \sigma_0^x \tau_i^x + h_i \tau_i^z \right).$$

where H_B is the Hamiltonian of the bath and σ_0^x pertains to a spin in the bath/ergodic grain at the boundary. The LIOM-spin τ_i^z is at distance *i* (in lattice units) from the ergodic grain, hence we set

$$g_i = \alpha^{i-1} g_1 \quad (\alpha < 1). \tag{24}$$

We take $\alpha = 3/4$, corresponding to inverse localization length $\zeta^{-1} = \ln(4/3)$. Since $\zeta^{-1} < \ln(2)/2$, our theory predicts that the crossover region extends to infinity: it should be able to thermalize an arbitrary amount of added LIOM spins.

We take $g_1 = 0.2$ and $h_i = 1 + h_i$ with h_i i.i.d. random variables drawn uniformly from [-0.5, 0.5]. These parameters

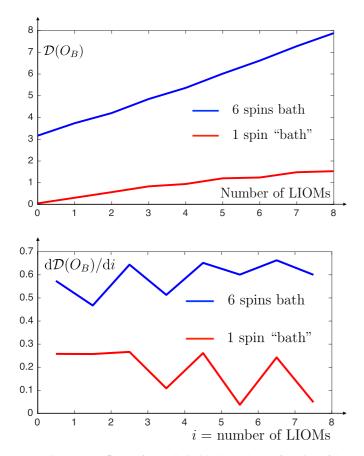


FIG. 3. (Top) $\mathcal{D}(O_B)$ for a spin inside the bath, as a function of the number of LIOMs coupled to the bath. In blue, a six-spin RM bath, N = 200; in red, a single spin bath, N = 4000. (Bottom) Discrete slopes of the above curves. At each $i + \frac{1}{2}$, we plot $\mathcal{D}(O_B, i + 1) - \mathcal{D}(O_B, i)$, with *i* the number of LIOMs.

should guarantee that the LIOM-spins τ_i are indeed by themselves localized degrees of freedom. This is a somewhat subtle statement because the τ_i are not coupled to each other and hence they have no mechanism for delocalization. However, we mean by this the interaction between them via the bath spin σ_0^x is not sufficient to delocalize them. In practice, this simply means that we check (see below) whether for a sufficiently small bath, the system is localized. For the bath, we first consider a grain of 6 spins with no particular spatial structure; H_B is then simply a random matrix (RM) acting on a 2⁶-dimensional space, with level spacing $1/\rho = 0.07$ and bandwidth 4.2. We couple up to 8 LIOMs to this grain. To minimize finite-size effects, we consider a bath spin operator $O_B = \sigma_B^x$ that is *not* the one used to couple to the LIOM's, i.e., not σ_0^x (it does not make sense to specify O_B as this bath has no spatial structure).

1. Strenghtening of the bath by the LIOMs

We focus first on a local operator inside the core of the ergodic grain. We compute the disorder-average of $\mathcal{D}(O_B)$, as a function of the number of LIOMs coupled to the bath. The result is represented by the blue line on the left panel of Fig. 3, while the corresponding slope of this curve is depicted on the

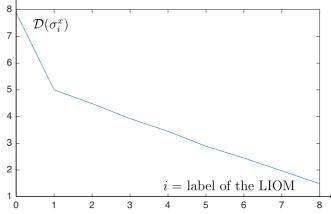


FIG. 4. $\mathcal{D}(\sigma_i^x)$ as a function of *i* for $0 \le i \le 8$, for a system of eight localized spins coupled to a sixspin RM bath. N = 200 for each point of the curve.

right panel. The value of this slope approaches the ideal value ln 2 predicted by our theory.

It remains to check that the spins τ_i are localized in the absence of the bath. For this, we replace the six-spin bath, by a single spin (bandwidth=2.25), for which perturbative computations predict the persistence of localization. We still compute the disorder-average of $\mathcal{D}(O_B)$, where O_B corresponds now to the unique spin in the bath. The result is represented by the red lines in Fig. 3. The slope much smaller than in the previous case (less than half of the ideal value) and we observe a tendency for the slope to decay.

2. The crossover region

We now turn to the investigation of the spatial dependence of ln IPR in the crossover region. Despite notational similarity, the quantity we consider is different from that on Fig. 3, where O was a bath operator and the dependence on i was simply because of the number of attached LIOM's. We now calculate $\mathcal{D}(\sigma_i^x)$ for all $0 \le i \le 8$ (where i = 0 corresponds to a spin inside the bath). Our theory, see Sec. IV, predicts that $\mathcal{D}(O_i) - \mathcal{D}(O_1), i \ge 1$ decays linearly with slope $2(\ln 4 - \ln 3) = 0.58$, whereas the decay from $\mathcal{D}(O_0)$ to $\mathcal{D}(O_1)$ is unrelated. The actual result of the calculation is depicted in Fig. 4. We indeed observe a linear decay from spin 1 to 8. The slope in the linear region is 0.5, which seems in reasonable agreement with the theoretical value 0.58.

B. A universal thermalization curve: comparison of different baths

In this section, we compare the action of different baths, differing in size and nature: random matrix, local Hamiltonian, and local Hamiltonian plus thermalized LIOM's. Already the fact that the latter can be labeled a bath is a nontrivial element and, in some sense, the core of the message of this paper. In our theory, the characteristics of the bath enter only via the dimensionless coupling constant \mathcal{G} and via the hybridization width w describing the thermalization of a spin. Moreover, if the FGR holds, then w is rigidly related to \mathcal{G} by $\mathcal{G}^2 = \rho w$, hence we focus on the dependence on \mathcal{G} here.

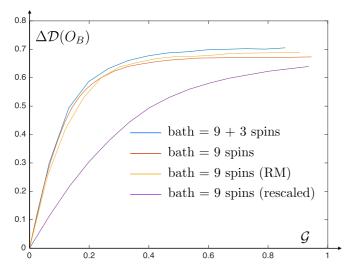


FIG. 5. $\Delta D(O_B) = D(O_B)|_{\mathcal{G}} - D(O_B)|_{\mathcal{G}=0}$ as a function of \mathcal{G} . (1) Blue: B' = 9 spins bath with local interactions and three thermalized LIOMs, N = 200 (the number of disorder realizations). (2) Orange: B' = 9 spins bath with local interactions, N = 1000. (3) yellow: B' = 9 spin RM bath, N = 100. (4) Purple: B' = 9 spins bath with local interactions and three unthermalized LIOMs.

The \mathcal{G} parameter enters our theory in deciding whether or not an external spin is thermalized. However, numerics shows that \mathcal{G} also accurately predicts the quality of the thermalization. This quality of thermalization is quantified by the increase in $\mathcal{D}(O_B)$ upon adding the spin, e.g.,

$$\Delta \mathcal{D}(O_B) := \mathcal{D}(O_B)|_{\mathcal{G}} - \mathcal{D}(O_B)|_{\mathcal{G}=0}$$

as a function of \mathcal{G} . Of course, $\Delta \mathcal{D}(O_B) = 0$ for $\mathcal{G} = 0$ and one expects that the effective dimension doubles by inclusion of the spin, hence $\Delta \mathcal{D}(O_B) \rightarrow \ln 2$ as $\mathcal{G} \gg 1$. The behavior for intermediate value of \mathcal{G} is in practice not so important for our theory. However, it is remarkable that the curves in Fig. 5 collapse rather well for different baths (the deviant lowest curve is explained below) and we feel it supports our theory in a compelling way.

Let us now discuss in detail the three different baths that we compare.

Local nine-spin bath plus three LIOMs We introduce a bath of nine spins with a local structure:

$$H_B = \sum_{i=1}^{9} \left(h'_i \sigma_i^z + J \sigma_i^x \right) + J' \sum_{i=1}^{8} \sigma_i^x \sigma_{i+1}^x \qquad (25)$$

with $h'_i = 1 + \tilde{h}'_i$ with $-0.3 < \tilde{h}'_i < 0.3$, J = 0.5, and J' = 1. We couple four LIOMs $\tau_{1,...,4}$ (we take h_i , $g_1 = 0.2$ and $\alpha = 3/4$ as in Sec. V A) to this bath, but we vary the coupling strength g_4 of the last one. So, the nine-spin bath plus three LIOMs form a bath, let us call it B', that we investigate by viewing how it acts on the fourth spin τ_4 . As explained above, this is done by measuring $\mathcal{D}(O_B)$ for an operator O_B in the original bath B. We choose $O_B = \sigma_4^x$ (this "four" refers to a site in the bath and is completely unrelated to the four of τ_4). Note that σ_9^x is the same as σ_0^x in Sec. V A.

We determine \mathcal{G} for the coupling of the fourth spin to B': $\mathcal{G} = g_4 \sqrt{v(2h_4)\rho}$ with $1/\rho$ the level spacing in B' and $v(\cdot)$ the structure factor of the bath operator σ_0^x . Numerically, we calculated \mathcal{G} as (the disorder average of) $g_4 \rho \sqrt{M}$ where

$$M := \frac{1}{\mathcal{N}} \sum_{b',s':|E(b',s')-E(b,s)| \leq 1} \delta_{s,-s'} \left| \langle b | \sigma_0^x | b' \rangle \right|^2$$

with \mathcal{N} the number of terms in the sum, b,b' eigenstates of the bath B', *s* an eigenstates of τ_4^z and b,s chosen so that $|b,s\rangle$ eigenstate with energy E(b,s) closest to 0 (maximal entropy).

Local nine-spin bath. Here we take the same nine-spin bath as above but without the three LIOMs coupled to it.

Random matrix. This is a random matrix bath mimicking the nine-spin bath (with dimension 2^9 and level spacing $1/\rho = 0.018$), no extra localized spins.

For contrast, we plot an example of a curve that doesn't match. The purple curve in Fig. 5 is built from the same data as the orange curve, but is scaled differently. Indeed, one considers here the case where there are actually three intermediate spins, as for the blue curve, but where these spins are uncoupled ($g_1 = g_2 = g_3 = 0$). It is thus clear that they have no physical effect, so that the data are the same as the one obtained on the orange curve; however, if one considers the original bath together with these three spins as the new bath B', one divides the level spacing by 2^3 , leading to a different definition of \mathcal{G} w.r.t. the orange curve. We see that the purple curve is clearly an outlier, indicating that when the three intermediate spins are truly coupled, they do participate to the thermalization of the last fourth spin.

Finally, we observe that the value of ΔD for the blue curve becomes even slightly larger than $\ln 2$ for values of \mathcal{G} close to 1. This is a priori surprising as the increase of dimension from a single spin should be ln 2 at most. We suspect the following scenario: before coupling the 4th spin, \mathcal{D} did not reach its maximal value, because the three coupled spins were only imperfectly thermalized. Indeed, in our numerics the bare values used for the first three spins are not so far from the critical value needed for thermalization. The first of these spins corresponds to $\mathcal{G} = 0.67$, which can still be considered slightly in the transition region, as is revealed by a careful inspection of the curves of Fig. 5. However, the situation becomes better for each added spin (this is a direct consequence of the fact that $\ln(4/3) > \ln 2/2$ and there is catchup effect: the fourth spin helps to complete the imperfect thermalization of the first three spins).

VI. CONCLUSION

We have proposed a simple RMT theory for the joint eigenfunctions of spins coupled to a finite bath. When we apply this theory repeatedly, we obtain a clear-cut prediction whether the system will be localized or ergodic. In this way, we investigate finite ergodic grain (bath) coupled to well-localized spins, i.e., with coupling strength small compared to disorder. The predictions are consistent with localization in d = 1 with exponentially decaying interactions: localization is stable with respect to such ergodic grains. For interactions that decay slower, or in d > 1, our theory predicts delocalization. The most quantitative result of our theory is a description of the spatial intermediate region between an ergodic grain and a d = 1 localized material. In particular, it states that any degree

of freedom, say a $\frac{1}{2}$ -spin, in this region enhances the ergodic grain, leading in particular to a doubling of the effective dimension or the IPR (inverse participation ratio) parameter. This prediction is reasonably validated by numerics, though there is need for finer tests. As an aside, the numerics reveals a rather universal pattern of thermalization that does not distinghuish between the action of a bath on very localized degrees of freedom or others, i.e., (nearly) ergodic degrees of freedom.

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APPENDIX A: NUMERICS ON THE HYBRIDIZATION WIDTH

We return to Sec. **II C** and we assume the notation used there. We test numerically the (FGR) relation

$$w \sim \frac{g^2}{\xi}.$$

We always choose the eigenstate ψ of the coupled system to lie in the middle of the spectrum, i.e., at E = 0 and consider mainly a random matrix (RM) bath, for which ξ is approximatively the full spectral width. The width w can depend a priori on ρ , ξ , g, and h, where we recall that ρ is the inverse of the level spacing (at maximal entropy). For the numerics below, we take h = 1 and g = 0.8. As long as 2h is significantly large than g, we do not expect any crucial dependence on h; this turns out to be so indeed (not shown).

Let us check that w is independent of ρ . For this, we fix g and h, and we consider four different RM baths, say B_1, \ldots, B_4 , acting on spaces with dimension from 2^8 to 2^{11} , rescaled in a such a way that ξ remains constant (the width is approximately equal to $\xi = 10$). The level spacing is the only variable parameter; it gets divided by 2 each time we change bath from B_1 to B_4 . The four corresponding hybridization curves are plotted on the upper panel of Fig. 6. The good matching of the curves indicate that w is indeed independent from ρ .

We next check that w depends on ξ as $1/\xi$. For this we repeat the previous numerics, rescaling now the baths so as to keep the level spacing constant (we take it approximately equal to $1/\rho = 0.02$) and varying ξ . Now the value of ξ gets doubled each time we change bath from B_i to B_{i+1} . To collapse the curves, we use the scaling relation. Since a Lorentzian distribution satisfies the scaling $\lambda f(\lambda x, \lambda w) = f(x, w)$, the relation $w \sim 1/\xi$ implies that the curves should collapse by plotting $2^{k-2} f_{B_k}(2^{k-2}x)$ instead of $f_{B_k}(x)$ (the hybridization

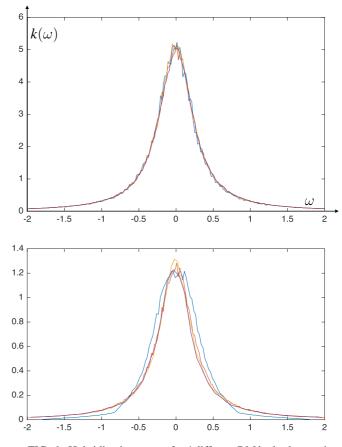


FIG. 6. Hybridization curves for 4 different RM baths, by varying the level spacing (upper panel) or the width (lower panel).

curves for the bath B_k) for $1 \le k \le 4$. The result is shown on the lower panel of Fig. 6. We observe again a good matching except for the blue curve corresponding to the smallest bath (k = 1); this discrepancy can be attributed to finite size effects and to the fact that the Lorentzian shape does not need to be strictly verified. Thanks to the two previous points, the dependence of w on g as $1/g^2$ now follows from dimensional analysis or simple rescaling of the parameters of the model.

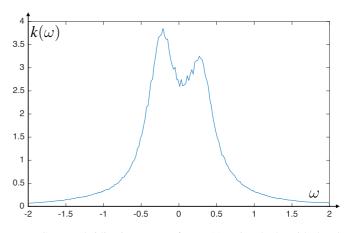


FIG. 7. Hybridization curve for a 11 spins bath with local interactions.

Finally, in Fig. 7, we show an example of an hybridization curve for an 11 spins bath with local interactions. The Hamiltonian of this bath is the same as the Hamiltonian in Eq. (25), with 9 and 8 above the summation signs respectively changed to 11 and 10. We observe a camel-like shape, showing that the Lorentzian distribution should only be taken as an idealization of the hybridization function [we also observe some asymmetry in the peaks, which however can be explained by noting that tr(H_B^{3}) \neq 0].

APPENDIX B: CALCULATIONS ON THE BACKREACTION

Here we carry out some calculations that were omitted in Sec. II E. First, we evaluate the kernel K(b,s|b',s') for b = b' in a weak-coupling approximation. To that end, we approximate the resolvent by its g = 0 value K_0 :

$$K_0(b,s|b,s') = g\langle b,s|\sigma_B^x \frac{1}{E' - H_0} \bar{P}'\sigma_s^x \sigma_B^x|b,s'\rangle$$

Since H_0 does not flip *s*, we can simplify $K_0(b,s|b,s') = \delta_{s,-s'}K_0(b,s|b,-s)$. Inserting a parition of unity, we write

$$\begin{split} K_0(b,s|b,-s) &= g \sum_{\tilde{b}} |\langle b|\sigma^x|\tilde{b}\rangle|^2 \frac{\chi(|\Delta| \ge w)}{\Delta} \\ &\approx \int d\omega \, \chi(|\Delta(\omega)| \ge w) \frac{gv(\omega)}{\Delta(\omega)}, \end{split}$$

where $\Delta \equiv \omega + 2sh + \{E(b, -s) - E'\}$ and we recall that term in $\{\ldots\}$ is restricted to $|\cdot| \leq w$. In the region where v has its bump, the integrand is typically of size $\frac{g}{\xi \max(h,\xi)}$, which leads to the estimate $\mathcal{W} \equiv \frac{g}{\max(h,\xi)}$ for the integral. If the function v were very rough around the cutoff singularity

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 $\Delta(\omega) = 0$, then this could change the estimate to $-W \ln W$, which does not affect the essence of our conclusion.

To get to the contribution to the structure factor (13), we return to the expression

$$\langle P\psi|\sigma_B^x|\bar{P}'\psi'\rangle = \sum_{b,b',s,s'} \langle P\psi|b,s\rangle K(b,s|b',s')\langle b',s'|P'\psi'\rangle.$$

Restricting to b = b', replacing K by K_0 and $\langle P\psi|b,s\rangle, \langle b',s'|P'\psi'\rangle$ by the random expressions from (10), we get the result by a central-limit calculation, as in Sec. II D.

As mentioned in Sec. II E, similar considerations also lead to a derivation of the FGR, which is phrased here as the fact that $||\bar{P}\psi|| \sim 1$, i.e., we are truncating the eigenstates exactly around their bump. Approximating the resolvent again by its lowest-order expression

$$ar{P}\psi pprox g \sum_{b,s} rac{\sqrt{k_0(\omega)\eta(b,s)}}{\sqrt{
ho}} rac{1}{E-H_0} ar{P}\sigma^x_S \sigma^x_B |b,s
angle$$

with $\omega = E - E(b,s)$, we can calculate (the expectation value of) $||\bar{P}\psi||^2$ as

$$||\bar{P}\psi||^2 \approx g^2 \sum_{b,s,b',s'} \frac{k_0(\omega)\chi(|\omega'| \ge w)}{(\omega')^2 \rho} |\langle b',s'|\sigma_B^x|b,s\rangle|^2,$$

where $\omega' = E - E(b', s')$. Plugging the ETH expression for the matrix elements of σ_{B}^{x} , we get

$$||\bar{P}\psi||^2 \approx g^2 \int \mathrm{d}\omega \mathrm{d}\omega' rac{k_0(\omega)\chi(|\omega'| \ge w)}{(\omega')^2} v(\omega'-\omega).$$

We use that $\int k_0 \sim 1$ (with width w) and we approximate v as a bump with width $\xi \gg w$ (FGR condition). Then the above integral yields indeed g^2/ξ . Most importantly, this conclusion is not affected if v had additional narrow peaks with small weight, cf. the splitting $v = v_{\rm sm} + v_{\rm irr}$ obtained in Sec. II E.

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