Many-body localization as a percolation phenomenon

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We examine the standard model of many-body localization (MBL), i.e., the disordered chain of interacting spinless fermions, by representing it as the network in the many-body (MB) basis of noninteracting localized Anderson states. Studying eigenstates of the full Hamiltonian, we find for strong disorders that the dynamics is confined to disconnected MB clusters. By simplifying the quantum problem to rate equations (RE) for MB states, in analogy with percolation problems, the MBL transition is located via the universal cluster distribution and the emergence of the macroscopic cluster. On the ergodic side, the RE well capture the diffusion transport, as found in the full quantum model. Still, we find for a broad intermediate range of parameters that the transport is anomalous, i.e., subdiffusive-like, emerging from weak links between MB states.

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Introduction. The interplay of disorder and interaction in dense fermionic systems remains a challenging theoretical problem, offering a novel scenario for a possible metal-insulator transition at elevated temperatures $T > 0$. While the (Anderson) localization of noninteracting fermions [1] is a well-established phenomenon in disordered systems, the role of interaction has been seriously theoretically addressed only within the last 15 years [2, 3]. Based mostly on numerical studies, the transition/crossover towards the many-body localization (MBL) has been revealed by several criteria: change of level statistics [3–6], slow growth of entanglement entropy [7–9], vanishing d.c. transport [10–16], absence of thermalization [17–19], where all these criteria may be related to the existence of a macroscopic number of integrals of motion in the MBL phase [20–24]. Importantly, qualitative features of the MBL have been found in several cold atoms experiments [25–28].

While model investigations of strongly disordered systems confirm the existence of the MBL, the phenomenology of the transient regime towards the normal diffusion is much less clear, making the physical interpretation of the interplay between interaction and strong disorder difficult. For the transient regime, there is abundant evidence for a subdiffusive nature of transport [12, 13, 29–31], accompanied with large and anomalous fluctuations of relevant quantum observables near the MBL transition [32, 33]. However, the existence of this transient regime and its origin is still under dispute [34–37]. As a plausible explanation, Griffith effects due to weak-link structures in real space have been proposed [12, 13, 18, 29].

In recent works, there is a growing number of numerical evidences emphasizing percolation aspects of the MBL transition, whereby the multifractal clustering appears in the many-body (MB) Fock space [9, 38–41], with implications for the both sides of the MBL transition.

In this Letter, we present numerical results for the prototype quantum MBL model that clearly reveals disorder-induced clustering effects. More precisely, we show that the basis consisting of localized MB states splits into disconnected clusters such that the dynamics of the system is confined to MB clusters up to very long times. These effects became even more evident in the formulation of the problem when quantum transitions are replaced by rate equations (RE). Such a RE approach has been recently applied by present authors to several quantum models of the propagation of (single) particles coupled to bosons [33, 42], revealing normal as well as subdiffusive transport behaviors. In the present case, the RE allows for a direct study of thermalization of MB charge-density. RE results are consistent with full quantum calculations, confirming nearly exponential decrease of diffusion with disorder strength. In the transient regime that spans over a broad range of parameters below the MBL transition, we find anomalous/subdiffusive relaxations towards the equilibrium, which can be attributed to weak links between MB states, with no apparent relation to the real-space weak-links.

Model in the Anderson MB basis and the RE approach. We consider the prototype model of MBL, with interacting spinless fermions in the disordered 1D system, equivalent to the XXZ spin-1/2 chain with random fields,

$$H = -t_h \sum_i (c_{i+1}^\dagger c_i + \text{H.c.}) + \sum_i \epsilon_i n_i + V \sum_i n_{i+1} n_i,$$

where the quenched local disorder is characterized by a uniform distribution $-W < \epsilon_i < W$. By setting $V = 2t_h$, we focus on the most frequently studied case of the isotropic Heisenberg chain, for which the MBL transition/crossover is expected at $W_c \sim 6 - 8$ [5, 14]. However, it should be noted that significantly larger values of $W_c$ have been reported recently as well [36, 43–46]. We use $t_h = 1$ as the unit of energy and focus on the half-filled case with $N = L/2$ fermions, where $L$ is the number of lattice sites.

In order to approach the problem from the localized side, we represent the model in the basis of single-particle And-
son states. In this representation, the noninteracting part of the Hamiltonian (1) is diagonal, $\hat{H}_0 = \sum_i \epsilon_i |\varphi_i\rangle \langle \varphi_i|$, while the interacting part takes the form, $\hat{H}' = \sum_{jklm} h_{jklm} |\varphi_j\rangle \langle \varphi_m| \varphi_k \langle \varphi_l|$. Depending on how many indices $jklm$ coincide, $H'$ may be divided in three parts, for which the explicit expressions are given in previous works [47, 48] and [49]. The Hartree-Fock term, $\hat{H}_F = \sum_{n>1} n_n |\varphi_n\rangle \langle \varphi_n|$, is diagonal in the Anderson MB basis and may be added to the noninteracting part, $H_0 = \hat{H}_0 + \hat{H}_F$, corresponding to energies $E_n^0$ of localized MB basis states $|\eta\rangle = |n_1=1, ..., n_L=L\rangle$. The remaining interacting part, $H' = \hat{H}_F' + \hat{H}_I'$, mixes different states $|\eta\rangle$, allowing for charge fluctuations.

When discussing the dynamics and real transitions between MB states inside or in the vicinity of MBL regime (as opposed to virtual ones, representing perturbative corrections), one should primarily consider those matrix elements between the MB states that satisfy the resonance condition (RC),

$$|H_{\eta\eta'}| > R(E_\eta^0 - E_{\eta'}^0), \quad H_{\eta\eta'} = \langle \eta | H' | \eta' \rangle,$$

with the RC parameter $R \lesssim 0.5$. The same reasoning is used for the reduced-basis approach [47, 48].

Making a step further by neglecting the quantum coherence of hopping between MB states, one can forget the relaxation from some initial MB occupation profile towards the equilibrium as a cascade of (irreversible) transitions, described by the RE for the MB occupations/probabilities, $p_\eta$,

$$\frac{d}{dt} p_\eta = \sum_{\eta' \neq \eta} \Gamma_{\eta\eta'} (p_{\eta'} - p_\eta) = \sum_{\eta'} \tilde{\Gamma}_{\eta\eta'} p_{\eta'},$$

satisfying $\sum_{\eta} p_\eta = 1$. Transition rates $\Gamma_{\eta\eta'} > 0$ take a Fermi-golden-rule (FGR) form, $\Gamma_{\eta\eta'} = \zeta |H'_{\eta\eta'}|^2 N_{\eta\eta'}$, with the MB density of states that is relevant for the transition,

$$N_{\eta\eta'} \sim \frac{R}{2|H_{\eta\eta'}|^2} \Theta \left( \frac{|H_{\eta\eta'}|^2}{2|H_{\eta\eta'}|^2} - |\Delta E_{\eta\eta'}^0| \right).$$

Although $\zeta$ does not influence any qualitative conclusions, to set the time scale in units corresponding to oscillations of two-level systems, we choose $\zeta = 1/(\pi R)$. On the other hand, the choice of $R$ directly influences the results, in particular the MBL transition value $W_c$. While the conservative RC would be $R = 0.5$, we use a bit softer cutoff $R = 0.3$.

**MB clustering and the percolation threshold.** Perfect clustering means that the Anderson MB basis, $|\eta\rangle$, may be split into disconnected sets (clusters) such that each MB eigenstate $|\mathcal{N}\rangle$ has a projection on a single cluster only. Such clustering can be univocally identified when $M_{\mathcal{N},\mathcal{N}'} = \langle \eta | \mathcal{N} | \eta \rangle$ is a block-diagonal matrix, whereby each block corresponds to a separate cluster. However, the eigenstates are typically sorted according to the energies, whereas the numbering of the MB basis is arbitrary. Therefore, in order to reveal such a block-diagonal structure, the rows and columns of $M_{\mathcal{N},\mathcal{N}'}$ should be permuted accordingly. To this end, we apply a simple sorting algorithm, based on an observation that for the eigenstates $|\mathcal{N}\rangle$ and $|\mathcal{N}'\rangle$ which belong to different clusters,

$$O(\mathcal{N}, \mathcal{N}') = \sum_{\eta} \langle \eta | \mathcal{N} | \eta \rangle \langle \eta | \mathcal{N}' | \eta \rangle,$$

vanishes. Starting from an arbitrary $|\mathcal{N} = 1\rangle$, we find $\max_{\mathcal{N}' \neq \mathcal{N}} O(\mathcal{N}, \mathcal{N}')$ and the resulting $|\mathcal{N}'\rangle$ is then considered as a consecutive eigenstate $|\mathcal{N} = 2\rangle$. The same procedure is repeated for each newly added state $|\mathcal{N}\rangle$, grouping in this way together the eigenstates belonging to the same cluster. In the second stage, we sort the basis states $|\eta\rangle$ according to their projections on already sorted eigenstates. That is, for each $|\mathcal{N}\rangle$ we find $\max_{\mathcal{N} \neq \mathcal{N}'} \langle \eta | \mathcal{N} | \eta \rangle$, which defines the place of $|\eta\rangle$ in the list, $n = \mathcal{N}$. How this algorithm works on the truncated Hamiltonian, with omitted non-resonant matrix elements, is shown in Fig. 1a for a strong disorder $W = 10$ and $L = 12$-site system. The block-diagonal structure of $M_{\mathcal{N},\mathcal{N}'}$ (and thus also the clustering) is fully apparent.

It remains to be checked that the clustering observed in Fig. 1a is not just an artifact of our truncation scheme in Eq. (2). To this end, we order the exact eigenstates of the full Hamiltonian according to the maximal projections $|\eta | \mathcal{N} | \eta \rangle$. For the basis states $\{|\eta\rangle\}$ we keep the ordering obtained for the truncated Hamiltonian. The result for the full Hamiltonian is shown in Fig. 1b for the same realization of disorder as in Fig. 1a. Although some exact eigenstates exhibit non-vanishing overlaps with the basis states in multiple clusters, one sees that the block structure of $M_{\mathcal{N},\mathcal{N}'}$ is present even when the RC is lifted. For the full Hamiltonian, we expect that an appropriately refined sorting may reveal an additional struct-
tured, e.g. multifractal properties [9, 38, 39, 41].

Considering the RC explicitly, the connectivity problem and distributions of clusters in the Fock space may be directly studied, with the onset of macroscopic cluster(s) being the natural criterion for the breakdown of the MBL. We introduce \( s = N_C/N_{MB} \), as the ratio of the cluster size, \( N_C \), and the total number of MB states, \( N_{MB} \), and look for universal behaviors related to the cluster sizes for the percolation-type of transitions. We start by analyzing the \( W \)-dependence of the relative volume of the Fock space associated to the maximal MB cluster, \( s_{\text{max}} \), evaluating typical averages, \( s_{\text{typ}}^{\text{mb}} = \exp(\log s_{\text{max}})_{\text{dis}} \), with \( \langle \ldots \rangle_{\text{dis}} \) representing the average over \( N_{\text{dis}} \) different disorder configurations. The numerical results for \( s_{\text{typ}}^{\text{mb}} \) as a function of \( W \) are shown in Fig. 2a, involving sampling over \( N_{\text{dis}} \geq 300 \) disorder configurations. Although the results exhibit a pronounced \( L \)-dependence of \( s_{\text{typ}}^{\text{mb}}(W) \) for all \( L \), it is important to notice from Fig. 2a that with the increasing \( L \) the drop of \( s_{\text{typ}}^{\text{mb}}(W) \) near the transition at \( W_c \approx 8 \) becomes sharper.

As a next step, we examine the probability distribution of MB clusters \( \mathcal{P}(s) \), which in the \( L \to \infty \) limit should be universal at the percolation transition \( W \approx W_c \) [50–52]. In particular, in Fig. 2b, we show the results in terms of the integrated distribution \( I(s) = \int_s^1 \mathcal{P}(s')ds' \), using the normalization \( I(s \to 0) = 1 \). The results in Fig. 2b are presented for the large system size \( L = 24 \) (\( N_{MB} \approx 3 \times 10^6 \)), averaging over \( N_{\text{dis}} \approx 50 \) samples. For \( W < W_c \), long plateaus exhibited by \( I(s) \) in Fig. 2b are consistent with the existence of a single macroscopic cluster. That is, the long plateaus that reach \( I(s = 1) \) as a straight line in Fig. 2b can be obtained only if one large cluster, \( s_{\text{max}} \approx 1 \), exists for each realization of disorder. The bending of \( I(s) \) near \( s = 1 \) for larger \( W \) indicates a degradation of the macroscopical cluster into a rapidly increasing number of small clusters as \( W \) increases, with sample-to-sample fluctuations of \( s_{\text{max}} \) due to finite \( L \) near the percolation transition. Because of these fluctuations, the probability of finding a macroscopic cluster above \( W_c \) remains finite, yet small (rare events), which is consistent with the very low values of \( I(s \approx 1) \) for \( W \gtrsim 8 \) in Fig. 2b. Near the percolation transition, the distribution becomes universal in a broad range of \( s \), exhibiting power-law behavior \( \mathcal{P}(s) \propto s^{-\xi} \). A simple fit for \( W = 8 \) gives \( \xi \approx 2.47 \), which is very close to the value 5/2 predicted for percolation models in high dimension \( (D > 6) \) [51, 53].

Charge-density relaxation. Recurrences on the real-space relaxations of the observed percolation phenomenon in the Fock space may be different. It this sense, our RE approach [33, 42, 47] in Eqs. (3) and (4) offers an important advantage, allowing for a study of dynamical relaxations and the thermalization on the lattice starting from nonequilibrium MB states. In particular, we analyze relaxations properties of the charge-density profile,

\[
\rho_q = \sum_n n_q p_n, \quad n_q = \sqrt{2 \over L} \sum_{i t} \cos(qt) |\phi_{ti}|^2 n_t, \quad (6)
\]

for the smallest \( q = \pi/L \) for systems with open boundary conditions. With the full diagonalization of \( N_{MB} \) linear RE in Eq. (3), we can express the density correlation function (DCF) \( C_q(t) = \langle \rho_q(t) \rho_{-q}^\alpha(t) \rangle \) in terms of eigenvalues \( \lambda_n \) and eigenfunctions \( w_{\alpha n} \),

\[
p_n = \sum_n c_n w_{\alpha n} e^{-\lambda_n t}, \quad \lambda_n w_{\alpha n} = -\sum_n \tilde{\Gamma}_{n\alpha} w_{\alpha n}. \quad (7)
\]

With a basis state as an initial nonequilibrium MB state, \( p_n^0 = \delta_{n\alpha_0} \), we get \( c_{\alpha} = w_{\alpha_0} \). The averaging over all initial states yields,

\[
C_q(t) = \frac{1}{N_{MB}} \sum_{\alpha > 0} |W_{\alpha}|^2 e^{-\lambda_n t}, \quad W_{\alpha} = \sum_n n_q w_{\alpha n}. \quad (8)
\]

where \( \lambda_{0} = 0 \) components are omitted, since they represent the equilibrium solutions, \( p_n = 1/N_C \), for each MB cluster. To discuss anomalous diffusion, we introduce a time-dependent diffusion given by,

\[
D(t) = -\left(1/q^2\right) d \left[ \ln C_q(t) \right]/dt. \quad (9)
\]

The full-diagonalization approach to the RE allows tracking of the dynamical solutions to arbitrary long times \( t \). Due to large \( N_{MB} \) it is restricted at present to \( L \leq 16 \) systems. Results presented in [49] for the regime \( 3 \leq W < W_c \) reveal a steady decrease of \( D(t) \) and absence of saturation even at very long times \( t \leq 10^4 \). For shorter \( t \leq 10^4 \), we employ direct time integration of the RE, Eq. (3), allowing for systems up to \( L = 24 \). To avoid infeasible sampling of the DCF over all initial states \( |\psi_0\rangle \), a convenient initial inhomogeneous distribution is chosen, \( p_n(t = 0) \propto \exp[-\tilde{\alpha}_q p_n] / T \), corresponding to a potential imposing an initial charge-density modulation \( (T = 0.5) \). A modified DCF is calculated next, \( \tilde{C}_q(t) = \langle \rho_{q}(t) \rangle / \langle \rho_{q}^0 \rangle \). Since the meaningful diffusion is allowed only in the macroscopic MB cluster, in the following we analyze only the latter.

In Fig. 3, typical \( \tilde{C}_q(t) \) are shown for \( L = 24 \) and \( N_{\text{dis}} = 50 \). For \( W > 2 \), it is rather evident that the DCF is not just a simple exponential one, expected for the normal diffusion, \( D(t) = \text{const} \). Indeed, the decays in Fig. 3 are
Figure 3. Typical DCF $\tilde{C}_q(t)$ for $L = 24$ system and various $W = 2 - 6$, obtained via time integration of the RE.

Figure 4. Integrated distribution of diffusion parameter $I(D)$, evaluated via the RE for $L = 24$ at different times $t$, for two different disorders $a) W = 2$ and $b) W = 5$. Presented are also corresponding full-quantum results (dashed curves), obtained for $L = 22$.

Figure 5. $a)$ Effective diffusion parameter $D_0$ and $b)$ the exponent $\beta$. Empty squares show results from typical $\tilde{C}_q(t)$ for $L = 24$ on Fig. 3, and filled squares from the median $D_m(t)$ as on Fig. 4a,b. In $a)$ we also plot $\tilde{D}$ (empty triangles) from full-quantum calculation on $L = 22$.

For $W = 5$ and small $D < 10^{-3}$ in Fig. 4b, discrepancies between the two approaches may be observed, which might originate from the fact that quantum result includes the whole system while the RE only macroscopic clusters. A quite uniform shifting of $I(D)$ along the logarithmic time scale in Fig. 4b is fully consistent with the stretched-exponential decay of DCF, namely $D_m(t) \sim D_0 (t_0/t)^{1-\beta}$, again with $\beta < 1$. It should be noted that for the disorder $W = 2$, as $L$ increases, we get $\beta \rightarrow 1$ and the normal diffusion $D(t) = D_0 = \text{const}$ is recovered. We expect that the most reliable values of $\beta$ and $D_0$ are obtained by considering the median $D_m(t)$. Namely, the estimate based on the typical $\tilde{C}_q(t)$ should be partially obscured by the very broad nature of $I(D)$ distributions.

Figure 5 summarizes the results of the RE approach for the two parameters $D_0$ and $\beta$, characterizing the anomalous transport behaviors in the transient regime, $2 < W < W_c$. The overall dependency of $D_0$ observed from Fig. 5a is exponential, i.e., $D_0 \propto \exp(-bW)$ with $b \sim 1.2$, while $\beta$ is approximately linear in $W$. In Fig. 5a, the effective $\tilde{D}$, obtained by the full-quantum calculations, is plotted by empty triangles, exhibiting the exponential dependence on $W$ as well. Here, we should remind of the relation between $\tilde{D}$ and d.c. conductivity $\tilde{\sigma}_0$, the latter being calculated for the same model in previous studies [10, 16], whereby at $T \gg W$ one gets $\tilde{\sigma}_0 = T \tilde{\sigma}_0 = \tilde{D}/4$, and essentially the same coefficient, $b \approx 1.1$ [16].

Conclusions. We have demonstrated that eigenstates of the strongly disordered MB system form a cluster-like structures, provided that in the present model eigenfunctions are expressed in the MB Anderson states. This effect becomes even more evident considering only MB matrix elements satisfying the resonant criterion. The emerging connectivity problem reveals the percolation threshold at critical disorder $W_c$, characterized by the vanishing of the macroscopic cluster and the universal distribution of cluster sizes. The location of $W_c$ depends on the resonance parameter $R$, which gives at chosen $R = 0.3$ very reasonable estimate, $W_c \sim 8$, consistent with the full-quantum calculations.

The charge dynamics (diffusion) studied in the context of...
the RE below the MBL transition even quantitatively agrees with the full-quantum results, with the exponential suppression of the effective diffusion constant with $W$. The diffusion is anomalous in the wide range, $2 < W < W_c$, being characterized by the dynamical exponent $\beta < 1$. Obtained anomalous diffusion indicates weakly coupled MB regions within the largest/macroscopic cluster, but with no evident/simple relation to the weak-link scenario in the real space.

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[49] See Supplemental Material at (link will be provided by publisher) where we present detailed description of the effective model, applied method and results for the full quantum model, and provide some additional results within the RE approach.

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