Exploring Localization in Nuclear Spin Chains

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Detailed Terms
Exploring Localization in Nuclear Spin Chains

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Characterizing out-of-equilibrium many-body dynamics is a complex but crucial task for quantum applications and understanding fundamental phenomena. A central question is the role of localization in quenching thermalization in many-body systems and whether such localization survives in the presence of interactions. Probing this question in real systems necessitates the development of an experimentally measurable metric that can distinguish between different types of localization. While it is known that the localized phase of interacting systems [many-body localization (MBL)] exhibits a long-time logarithmic growth in entanglement entropy that distinguishes it from the noninteracting case of Anderson localization (AL), entanglement entropy is difficult to measure experimentally. Here, we present a novel correlation metric, capable of distinguishing MBL from AL in high-temperature spin systems. We demonstrate the use of this metric to detect localization in a natural solid-state spin system using nuclear magnetic resonance (NMR). We engineer the natural Hamiltonian to controllably introduce disorder and interactions, and observe the emergence of localization. In particular, while our correlation metric saturates for AL, it slowly keeps increasing for MBL, demonstrating analogous features to entanglement entropy, as we show in simulations. Our results show that our NMR techniques, akin to measuring out-of-time correlations, are well suited for studying localization in spin systems.

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Anderson first demonstrated that single particle wave functions can become exponentially localized in the presence of disorder [1]. Whether this localization [2–4] survives in the presence of interactions has received much attention in recent years [5–10]. Numerical evidence in spin chains indicates that the system may be in the many-body localization (MBL) or ergodic phase depending on the relative strength of interaction and disorder [11–13]. MBL can be distinguished from its noninteracting counterpart [Anderson localization (AL)] via the dynamics of entanglement entropy [14–17]. Entanglement entropy (EE) is, however, difficult to evaluate experimentally and so far has only been measured on systems with a small number of particles [18]. One way to circumvent this challenge is to measure entanglement witnesses such as the quantum Fisher information, which can serve as a lower bound for entanglement entropy [8] for pure states.

A remarkable feature about the MBL phase is that it is predicted to persist at high and even infinite temperature [19], where states are highly mixed and there is little to no entanglement present. How does one characterize the MBL phase experimentally in such a system? Here, we introduce a novel metric capable of distinguishing MBL from AL in the nonequilibrium dynamics of highly mixed states and provide both numerical and experimental evidence in support. Our approach requires no local control and relies only on collective rotations and measurements, in contrast to recently proposed metrics [20] that also detect the spread of correlations, but require single-spin addressability. The experimental system is composed of nuclear spins in a natural solid-state system with high fidelity to an ensemble of 1D, nearest-neighbor coupled spin chains [21,22]. We exploit Hamiltonian engineering techniques to selectively introduce and tune both the interaction strength and the degree of disorder in the system, and measure the growth of many-spin correlations in both the AL and MBL regimes.

We consider a linear chain of \( L \) spins initially at equilibrium at high temperature \((\beta \rightarrow 0)\) in a strong magnetic field aligned along the \( \hat{z} \) direction. Under these conditions, the thermal equilibrium state of the system can be expressed \( \rho_{\text{eq}} = (1 - e^{-\beta}) S_{z} / 2 \) (with \( S \) as the spin-1/2 operator) to first order in \( e = \beta \omega_{L} \ll 1 \), where \( \omega_{L} \) is the spin Zeeman energy and \( \hbar = 1 \). Any spin-spin interactions are assumed to be negligible compared to the Zeeman energy, so that the natural interaction Hamiltonian commutes with the thermal equilibrium state.

If the effective interaction Hamiltonian \( H \) of the system is changed suddenly (a rapid quench), the system is no longer in equilibrium and evolves into a many-body correlated state. The presence of disorder hinders the growth of correlations and can give rise to localized states, characterized by an exponentially decreasing probability of...
correlations outside a typical localization length $\xi$, as shown in Fig. 1. Inspired by this picture, we define a metric of localization that measures the average length over which correlations have developed.

We can generically write the high-temperature time-evolved density matrix as

$$\rho(t) = \frac{\rho_0}{2^L} - \frac{e^{-L}}{2^L} \sum_{k=1}^{\xi} \sum_{l=1}^{\xi} b_k^{(l)}(t) B_k^{l*},$$

where $B_k$ are operators composed of tensor products of $k$ Pauli matrices and $L - k$ identity operators. Here, $\xi$ is the number of configurations with exactly $k$ nonidentity Pauli operators. To quantify localization we define the “average correlation length”

$$L_c = \sum_{k=1}^{\xi} k f_k,$$

where $f_k = \sum_{i=1}^{\xi} |b_k^{(i)}|^2$ is the contribution of all possible spin correlations with Hamming weight $k$ (with $\sum_{k=1}^{\xi} f_k = 1$). In the initial equilibrium state $\rho_0$ there are no spin correlations and $L_c = 1$. In the absence of disorder, we expect $L_c$ to grow and eventually saturate at a value dependent on $L$. Introducing disorder leads to a quantitatively different behavior. When the system is noninteracting, AL leads to a coherent suppression of many-spin correlations and $L_c$ is bound by the localization length $\xi$. When interactions are present, disorder is unable to completely suppress the correlation growth. The slow growth of $L_c$ in the presence of interactions is the key feature that enables $L_c$ to distinguish between AL and MBL for mixed states.

Consider an effective spin Hamiltonian of the form

$$H = \frac{u + \frac{1}{2}}{2} \sum_{j=1}^{L-1} JS_j^x S_{j+1}^x + \frac{v}{2} \sum_{j=1}^{L-1} JS_j^y S_{j+1}^y + g \sum_{j=1}^{L} h_j S_j^z - \frac{1}{2} \sum_{j=1}^{L-1} JS_j^z S_{j+1}^z.$$

The first two terms represent an integrable Hamiltonian, as they map to a free fermionic Hamiltonian via a Jordan-Wigner transformation [23]. The third term corresponds to on site disorder, and the last term introduces interactions between fermions (see Sec. 2 in the Supplemental Material [24], which includes Refs. [25–41]). Tuning the relative strength of these parameters allows us to explore different physical regimes. Figure 2 shows that both EE ($S = -\text{Tr}(\rho_L \log \rho_L)$, where $\rho_L$ is the reduced density matrix of the left half of the chain) and the correlation length $L_c$ display a characteristic logarithmic growth in time [15] when the system enters the MBL phase and saturate when the system is noninteracting. These numerical simulations suggest that $L_c$ can be used as an alternative to EE to distinguish MBL from AL for mixed states (Sec. 6.3 of the Supplemental Material [24]). $L_c$ and EE are related for more general states that arise from evolution under other spin Hamiltonians.

Measuring $L_c$ for a generic many-body state is challenging, since it is usually difficult to directly measure many-body correlations to determine $f_k$, and the number of configurations $\xi$ is exponential in $k$ and $L$. Here, we show how to extract $L_c$ in our experiments, with a method that can be extended to other systems.

Our experimental system consists of a single crystal of fluorapatite [Ca$_5$(PO$_4$)$_3$F] placed in a strong magnetic field ($7$ T, $\omega_L = 283$ MHz). The $^{19}$F spin-1/2 nuclei in the hexagonal fluorapatite crystal form linear chains along the $c$ axis, interrupted only by rare defects, each surrounded by six other chains. When the $c$ axis is oriented parallel to the external magnetic field, the cross-chain couplings is 40 times weaker than nearest-neighbor intrachain couplings ($J = -33$ krad/sec). The system can then be treated approximately as an ensemble of identical spin chains.
in 1D systems, we find instead a practical experimental dipolar Hamiltonian, \( H_{\text{nat}} = \frac{1}{2} \sum_{j<k} J_{jk} (2 S_j^x S_k^x - S_j^z S_k^z) + \sum_j h_j S_j^z, \)
where \( h_j \) is now a random variable representing the disordered field seen locally by each \(^1^H^F\) nucleus. The dipolar coupling between \(^3^P\) nuclei is about 27 times smaller than that between \(^1^H^F\) nuclei and can be neglected on our experiment time scales.

At room temperature, the P spins are in an equal mixture of \( m_e = \pm 1/2 \) states. This allows us to replace the heteronuclear interactions by \( \sum_j h_j S_j^z \), where \( h_j \) is a random variable representing the disordered field seen locally by each \(^1^H^F\) nucleus. The dipolar coupling between \(^3^P\) nuclei is about 27 times smaller than that between \(^1^H^F\) nuclei and can be neglected on our experiment time scales.

The random local field thus appears quasistatic in these experiments, resulting in an effective Hamiltonian \( H_{\text{nat}}^{\text{eff}} = (J/2) \sum_j (2 S_j^x S_j^{x+1} - S_j^z S_j^{z+1} - S_j^{z-1} S_j^{z+1}) + \sum_j h_j S_j^z \), where we kept nearest-neighbor couplings only.

While the high-temperature thermal equilibrium state does not evolve under this Hamiltonian, we can quench the system to a different effective Hamiltonian of the form of Eq. (3) by periodically applying a radio frequency (rf) pulse sequence in resonance with the F spins. This method (called coherent averaging [44]) has been long used in the nuclear magnetic resonance (NMR) literature for spectroscopy and condensed matter studies. Here, we further push these techniques to engineer the broad class of Floquet (periodic) Hamiltonians in Eq. (3), with tunable disorder and interactions. Changing the sequences of pulses and delays in a period, we can experimentally adjust the parameters \( u, v, \) and \( g \) and explore various regimes of interest (Sec. 3.2 in the Supplemental Material [24] shows the experimental pulse sequence). In addition, we are also able to reverse the arrow of time, a tool that allows measuring out-of-time ordered correlations (OTOCs).

In order to calculate the correlation length \( L_c \), we need the coefficients \( f_k \), which we can determine experimentally by borrowing from well-known NMR techniques that approximate the number of correlated spins by their quantum coherence number [45]. Multiple quantum coherence (MQC) intensities of order \( q \) describe the contribution of terms \( |m_a\rangle \langle m_b| \) in the density matrix, such that \( m_a - m_b = q \), with \( m_a \) the collective \( S_a \) eigenvalue (typically \( a = z \)). MQC intensities \( I_q \) can be measured by relying on their distinct behavior under collective rotations [45–47]. The distribution of \( I_q \) has been traditionally used to approximate the average number of correlated spins in 3D spin networks [48–50]. While this approximation fails in 1D systems, we find instead a practical experimental protocol to exactly measure \( L_c \) for noninteracting systems. The protocol still yields a very good approximation for disordered interacting (MBL) systems.

We first note that, in noninteracting systems, for simple initial states such as \( \rho_{\text{eq}} \), the density operator at time \( t \), when expanded in the form of Eq. (1) has a particularly simple form. The number of configurations with \( k \) Pauli operators, \( \zeta_k \propto L - k \), as all many-spin correlations are of the form \( B_k \sim S_a^z (\prod_{i=1}^{k-1} S_i^z) S_b^z (\prod_{i=k}^{L-1} S_i^z) \), where the end spins \( S_{a,b}^z \) are either \( S_a \) or \( S_b \). This structure is key to extracting the \( f_k \) coefficients, as correlations with different \( k \) will exhibit distinct MQC intensities. To further distinguish the four different end-spin combinations, we first decompose \( \rho(t) \) into four corresponding orthogonal blocks, using time reversal and phase cycling [51], and then measure the MQC intensities encoded in the \( x \) axis for each \( j \)th block, \( I_q^j \) (see Sec. 5 in the Supplemental Material [24]). The resulting MQC intensities can be related to \( f_k \) in Eq. (2) by a linear transformation, \( f_k = \sum_q I_q^j \), and from the extracted \( f_k \) we can calculate \( L_c \). While this protocol was designed for the Hamiltonian we investigated, similar strategies will be available for other integrable Hamiltonians, with a proper choice of the axes along which the MQC are measured.

As long as the interaction term is not too large (and disorder large enough), we expect the evolved density matrix state to still mostly contain the simpler many-spin correlations described above, thus allowing us to extract an approximate \( L_c \). The validity of this argument can be seen from the simulation results shown in Fig. 2, where the approximated \( L_c \) (calculated from the MQC) continues to closely track the exact \( L_c \) and the entanglement entropy in the MBL phase.

Combining Hamiltonian engineering with MQC readout, we can explore the behavior of both noninteracting and interacting models in the presence of disorder. Figure 3 shows the experimentally extracted \( L_c \) for our interacting model, as compared to the noninteracting case. For the noninteracting Hamiltonian \( (v = 0) \), in the absence of disorder, we expect \( L_c \) to increase linearly, consistent with...
the Lieb-Robinson bound for short-ranged Hamiltonians [52]. In the thermodynamic limit $L \to \infty$ and at large times $uJt \gg 1$, $L_c$ grows with a velocity $V = 2uj/\pi$. In the presence of disorder, instead, we expect $L_c$ to initially increase, as spins correlate within the localization length, and to saturate at long times due to AL. This experimental evidence proves that our Hamiltonian engineering technique can indeed introduce disorder in the system evolution. The figure also shows the behavior of $L_c$ as the strength of the interactions $\{u, v\}$ in Eq. (3) are varied, for a fixed disorder strength. The experiments clearly reveal the emergence of slow growth in $L_c$ when interactions are added, the hallmark feature of MBL [15,53].

The strength and limitations of our experimental system are evident when we consider the change in $L_c$ as a function of disorder strength for the noninteracting case (Fig. 4). Increasing disorder is clearly seen to result in a saturation of $L_c$, consistent with AL. The lines are numerical simulations, showing that experimental results are consistent with theoretical predictions. Discrepancies at higher $L_c$ are likely due to experimental imperfections.

Control imperfection (such as pulse errors and rf transients) and decoherence due to the open system dynamics preferentially affect the higher quantum coherence of large spin correlations, leading to an apparent saturation of $L_c$. The same experimental imperfections make it even more difficult to observe the ergodic phase, where interactions dominate disorder, ideally leading to a fast growth in time of the correlation length, which is more heavily affected by the observed saturation. While high-fidelity experimental control of complex many-body states is key for any experimental metric of complexity, in some cases, it is still possible to distinguish between the saturation of $L_c$ due to experimental limitations at long time and its quenching due to increasing disorder using additional symmetry properties of the MQCs (see Sec. 5 in Supplemental Material [24]).

Note that in the experiments we can probe this dynamics only for relatively short times, where the physical system is a good approximation to the ideal model, as verified elsewhere [21]. Indeed, while the average chain length (determined by crystal defects) is much longer than the 20–25 spins explored on these time scales, we have long-range couplings ($\propto 1/r^3$) in a 3D crystal, where each spin chain interacts with six surrounding chains. In addition, pulse imperfections and higher orders in the Magnus expansion can lead to unwanted terms in the engineered Hamiltonian. We note that rapidly applied rf pulses do not give rise to heating [54], while the unavoidable interaction with the environment, dominated by other spins in the system, leads to decoherence (dephasing) that affects equally the interacting and noninteracting regimes. We kept the experimental time short to minimize these effects and observe the localization regime, before the experimentally unavoidable thermalization can appear (indeed the time is also much shorter than the relaxation time $T_1 \approx 0.8$ s and the P dynamics).

We can obtain a more intuitive understanding of why our experimental method for extracting the correlation length from MQC is quite robust. While measuring $L_c$ via the MQC is exact in the integrable case, this method can still be applied to MBL systems due to their “emergent integrability,” characterized by a complete set of local integrals of motions (LIOMs) [16,17]. While the number of possible configurations $\zeta_k$ in these LIOMs is exponential, only a fraction of them (corresponding to small $k$) have significant weights—a consequence of area law entanglement in MBL systems [55,56]. Then, when applied to MBL systems, the MQC method approximately counts the $L_c$ of these interacting LIOMs, while still exhibiting the same logarithmic growth as entanglement entropy. We can further understand our measurement in terms of OTOCs [32,57,58]. As explained in detail in Sec. 4 of the Supplemental Material [24], in order to extract the MQC intensities we effectively measure the quantities

$$S_{\phi}(t) = \text{Tr}[\rho_{eq}\Phi(t)\rho_{eq}\Phi(t)\rho_{eq}].$$

with

$$\Phi(t) = U(t)e^{i\delta \sum_j S_j U^t(t)}.$$

![FIG. 4. Experimental correlations in noninteracting spin chains. Correlation length $L_c$ for various strength $g$ of disordered transverse fields, with $u = 0.24$ and $v = 0$ [Eq. (3)]. Errorbars are determined from the noise in the free induction decay. The lines are numerical simulations using 6 (solid), 10 (dotted), and 40 (dashed) spins, respectively, averaged over 126 disorder realizations.](image-url)
In conclusion, we introduced a novel metric for localization, able to distinguish between many-body and single-particle localization. The correlation metric can be measured experimentally, with the only requirement of collective rotations and measurements, by extending MQC techniques developed in NMR (which can as well be applied to many other physical systems [58]). We also reveal an interesting relationship between the protocol for measuring the correlation length and the measurement of OTOCs, thus further confirming its ability to measure the logarithmic growth of entanglement associated with MBL. Thanks to our control techniques, we were able to explore a broad range of interesting behaviors in this solid-state spin system. In particular, we observed, for the first time, many-body localization in a natural spin system associated with a single crystal at high temperature. We note that, while we interpreted our results mostly based on a simplified model (1D, nearest-neighbour couplings), the real system is more complex due to long-range interactions and a 3D structure. It will be thus interesting to use the tools developed in this work to study subtler properties of localization when these effects are highlighted by the experimental scheme.

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