Relationship between initial state and Hamiltonian as a main factor for thermalization

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We explore the role played by the initial state on the onset of thermalization in isolated quantum systems. If the initial state has a chaotic structure with respect to the Hamiltonian dictating its evolution, i.e., if it fills the energy shell ergodically, thermalization is certain to occur. This happens when the initial state is an eigenstate of a full random matrix and the eigenstates of the Hamiltonian are delocalized. In this case, the results for the observables are equivalent to those obtained with thermal states at infinite temperature. However, finite real systems with few-body short-range interactions are deprived of fully extended eigenstates, even when described by a non-integrable Hamiltonian. We examine how the observables in such real systems, be the model integrable or chaotic, approach thermal averages as the initial state gets closer to the middle of the spectrum, where it gets more delocalized. Our numerical studies are based on initial states with energies that cover the entire lower half of the spectrum of one-dimensional Heisenberg spin-1/2 systems.

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I. INTRODUCTION

Experiments in optical lattices have enhanced the interest in the non-equilibrium dynamics of isolated quantum systems \cite{1,2}. New breath has been brought, for example, to the old pursuit of deriving thermodynamics from first principles. One of the main questions in this context refers to the conditions for an isolated quantum system initially far from equilibrium to reach thermal equilibrium. How decisive are regimes, initial states, and observables? What is universal?

A general picture has been developed associating chaos with the onset of thermalization \cite{3,11}, but several examples have been promoted as violations of this picture. Cases have been presented of chaotic Hamiltonians where thermalization was not observed for certain initial states \cite{12,16} and of integrable systems where thermalization appeared to be reached \cite{17,22}.

It is important to emphasize that the mere appearance of signatures of chaos associated with the bulk of eigenvalues, such as level repulsion or rigidity \cite{22}, is not sufficient for the onset of thermalization for any initial state. Real systems have few-body and usually short-range interactions. Contrary to full random matrices, their density of states has a Gaussian shape \cite{24,25} and their delocalized eigenstates are restricted to the middle of the spectrum \cite{3,7,24,28}. If the initial state has energy close to the edges of the spectrum, the main contributions to its evolution may come from localized eigenstates and thermalization may not occur.

In full random matrices, the eigenstates are completely extended pseudo-random vectors. In real chaotic systems, even in the middle of the spectrum, the eigenstates are limited by the energy shell and their components may show correlations \cite{29}. Yet, if the initial state is close to the middle of the spectrum, thermalization is expected to happen. Thermalization requires a substantial sampling of delocalized eigenstates, but the latter do not need to be completely extended. It is then natural to presume that thermalization could happen also for integrable Hamiltonians with delocalized eigenstates, provided the initial state be nearly chaotic.

The reasoning above shows a change in perspective with respect to the condition for thermalization, putting emphasi-
Thermalization implies that the expectation value of the observable is close to the thermal average most of the time. This holds under two essential conditions:

(1) The fluctuations of $\langle \hat{O}(t) \rangle$ about the infinite time average are small and vanish in the thermodynamic limit. We can then talk about equilibration in a probabilistic sense. The rate of decay of these fluctuations with system size depends on the system investigated \cite{35, 12}. The important fact for us here is that for the models we study the temporal fluctuations are indeed small and should vanish for very large systems.

(2) The infinite time average and the thermal average are very close in finite systems and eventually coincide in the thermodynamic limit,

$$\langle \hat{O} \rangle_{\text{DE}} = \langle \hat{O} \rangle_{\text{ME}}.$$  

Above,

$$\langle \hat{O} \rangle_{\text{ME}} = \frac{1}{N_{E^m, \Delta E}} \sum_{\alpha \atop |E^m - E_{\alpha}| < \Delta E} O_{\alpha \alpha},$$  

is the microcanonical average, which is appropriate when dealing with isolated systems. $N_{E^m, \Delta E}$ stands for the number of energy eigenstates in the window $\Delta E$, the latter is sufficiently small compared with the energy spectrum, but large enough to contain many energy states, and $E^m$ is the mean energy of the initial state.

The DE depends on the initial state via the components $|C_{\alpha \alpha}|^2$, while the ME depends only on the energy. For initial states narrow in energy \cite{43}, two scenarios may lead to the proximity between the two ensembles:

(i) The eigenstate expectation value of the observable, $O_{\alpha \alpha}$, is a smooth function of energy. When the values of $O_{\alpha \alpha}$ do not fluctuate for states close in energy, the result from a single eigenstate inside the microcanonical window agrees with the microcanonical average. This is the point of view of the Eigenstate Thermalization Hypothesis (ETH) \cite{3, 4, 11, 14, 44, 46}, which certainly holds when the eigenstates of the system are random vectors. Computing $O_{\alpha \alpha}$ with one or another random state leads to very similar results. However, for realistic chaotic systems, as already mentioned, this can happen only in the middle of the spectrum, where we can find nearly chaotic eigenstates.

(ii) The coefficients $|C_{\alpha \alpha}|^2$'s behave as random variables. Their fluctuations are uncorrelated with possible fluctuations of $O_{\alpha \alpha}$. In Eq. (3), we can then deal with the average of $|C_{\alpha \alpha}|^2$ \cite{47, 48}. This condition is more general than (i). It incorporates (i) when $\hat{H}_F$ is chaotic and the initial state is close to the middle of its spectrum, but it allows also for thermalization under an integrable $\hat{H}_F$ depending on the initial state.

III. ENERGY SHELL

The notion of energy shell is often used in quantum chaos. The usual procedure in the field is to separate the total Hamiltonian in an unperturbed part, which describes the non-interacting particles (or quasi-particles), and a perturbation,
which represents the inter-(quasi-)particle interactions and may drive the system into the chaotic domain. The Hamiltonian matrix is written in the basis corresponding to the unperturbed vectors, which constitute the mean-field basis.

A mean-field basis vector $|n\rangle$ projected on the eigenstates $|\psi_{\alpha}\rangle$ of the total Hamiltonian is written as

$$|n\rangle = \sum_{\alpha} C^n_{\alpha} |\psi_{\alpha}\rangle.$$

The distribution of the components $|C^n_{\alpha}|^2$ in the eigenvalues $E_{\alpha}$ is known as the strength function or local density of states [49]. The energy shell corresponds to the maximal spreading of the initial state is given by a Gaussian centered at

$$\langle E_{\text{ini}} \rangle = \sum_{\alpha} |C^{\text{ini}}_{\alpha}|^2 E_{\alpha} \quad (6)$$

and of variance

$$\sigma^2 = \sum_{\alpha} |C^{\text{ini}}_{\alpha}|^2 (E_{\alpha} - \langle E \rangle)^2$$

$$= \sum_{\alpha} \langle \hat{H}_F | n \rangle \langle n | \hat{H}_F | \text{ini} \rangle - \langle E^{\text{ini}} \rangle^2 \quad (7)$$

$$= \sum_{n \neq \text{ini}} |H_{\text{ini},n}|^2.$$

The variance of the energy shell corresponds to the energy distribution of the initial state. It depends only on the sum of the square of the off-diagonal elements of the final Hamiltonian $[8]$. The values of $E^{\text{ini}}$ and $\sigma$ are straightforward to obtain when $\hat{H}_F$ is already in a diagonal form or trivially solved [55].

To quantify the level of delocalization of the initial state we use the inverse participation ratio,

$$\text{IPR}^{\text{ini}} = \frac{1}{\sum_{\alpha} |C^{\text{ini}}_{\alpha}|^4}. \quad (8)$$

If the initial state is an eigenstate of a full random matrix from a Gaussian Orthogonal Ensemble (GOE) [23], its projection on the eigenstates of the systems we study here is again a GOE-type of vector, with probability amplitudes from a normal distribution. In this case, $\text{IPR}^{\text{ini}} \sim D/3$ [50], where $D$ is the dimension of the Hamiltonian matrix. If the eigenstate comes from a Gaussian Unitary Ensemble (GUE), the projection is again a GUE-vector and, as we verified, $\text{IPR}^{\text{ini}} \sim D/2$. Both states fill the energy shell ergodically.

It has been shown that a state corresponding to a random superposition of Ising states manifests thermal features. Specifically, the results for local observables led to the same outcomes obtained with a mixed state at infinite temperature [34, 51, 52]. The state is constructed so that the probability amplitudes of the basis vectors have all the same absolute value, $1/\sqrt{D}$, but differ by a random phase $e^{i2\pi\varphi}$, where $\varphi$ is a uniformly distributed random variable in $[0, 1]$. We have checked that the projection of such a state onto the eigenstates of our spin-1/2 Hamiltonians leads to vectors very similar to GUE eigenstates, with $\text{IPR}^{\text{ini}} \sim D/2$.

We infer that an initial state with $C^{\text{ini}}_{\alpha}$’s randomly distributed, as the coefficients of eigenstates from full random matrices, have properties similar to those of thermal states at infinite temperature. This is expected, since on average $|C^{\text{ini}}_{\alpha}|^2$ equals $1/D$. We have indeed confirmed that, for the observables studied here, when the initial state is an eigenstate from a GOE,

$$\langle \hat{O} \rangle_{\text{DE}} \sim \langle \hat{O} \rangle_{T \rightarrow \infty}, \quad (9)$$

where $T \to \infty$ indicates the result for a thermal state $\rho$ at infinite temperature, $\rho = \sum_{\alpha} |\psi_{\alpha}\rangle \langle \psi_{\alpha}|/D$.

The initial states considered in this work come from Hamiltonians which, as those from GOE’s, are real and symmetric. But since our $\hat{H}_I$ and $\hat{H}_F$ have only two-body short-range interactions, none of our initial states can reach maximum delocalization with $\text{IPR}^{\text{ini}} \sim D/3$. This does not discard, however, the possibility of having infinite time averages approaching microcanonical averages.

**IV. MODEL AND QUENCHES**

We consider a one-dimensional system with open boundary conditions composed of $L$ coupled spins-1/2 and described by the Hamiltonian,

$$\hat{H} = \hat{H}_z + \hat{H}_{\text{NN}} + \lambda \hat{H}_{\text{NNN}}, \quad (10)$$

where

$$\hat{H}_z = \epsilon \hat{S}_z^i$$

$$\hat{H}_{\text{NN}} = J \sum_{i=1}^{L-1} \left( \hat{S}_z^i \hat{S}_z^{i+1} + \hat{S}_y^i \hat{S}_y^{i+1} + \Delta \hat{S}_z^i \hat{S}_z^{i+1} \right),$$

$$\hat{H}_{\text{NNN}} = J \sum_{i=1}^{L-2} \left( \hat{S}_z^i \hat{S}_z^{i+2} + \hat{S}_y^i \hat{S}_y^{i+2} + \Delta \hat{S}_z^i \hat{S}_z^{i+2} \right).$$

Above, $\hat{S}_{x,y,z}^i$ are spin operators acting on site $i$. $\hat{H}_z$ indicates the presence of a defect on the first site of the chain. It is generated by applying a magnetic field in the $z$-direction, which is slightly larger than the magnetic field on the other sites. The coupling between nearest neighbors (NN) is given by $\hat{H}_{\text{NN}}.$
which contains the flip-flop term $\hat{S}_x^i \hat{S}_x^{i+1} + \hat{S}_y^i \hat{S}_y^{i+1}$ and the Ising interaction $\hat{S}_z^i \hat{S}_z^{i+1}$. $\hat{H}_{\text{NNN}}$ describes the coupling between next-nearest neighbors (NNN). $\Delta$ is the anisotropy parameter and $\lambda$ refers to the ratio between NNN and NN exchange, both are assumed positive. The exchange coupling constant $J$ determines the energy scale and is set to 1.

When both parameters $\Delta$ and $\lambda$ are simultaneously equal to zero, $H$ describes the XX model and can be mapped onto a system of noninteracting spinless fermions, being trivially solvable [53]. When $\lambda = 0$ and $\Delta \neq 1$, we have the XXZ model, which is still integrable but now solved by means of the Bethe ansatz [54]. When $\lambda \neq 0$ the system is non-integrable and may become chaotic [55, 56]. Notice that we refer here to the XX and the XXZ Hamiltonian when only NN couplings are present, so both cases correspond to integrable models.

The purpose of the small defect on the first site of the chain is to break trivial symmetries, such as parity, conservation of total spin, and spin reversal [57, 58], without breaking the integrability of the system [59]. We fix $\epsilon = 0.1J$. Conservation of total spin in the $z$-direction, $\hat{S}^z = \sum_n \hat{S}_n^z$, is a remaining symmetry. We deal with the subspace that has $L/3$ up-spins, implying dimension $D = L!/(2L/3)!L/3)!$ and $\hat{S}^z = -L/6$.

Four quenches are investigated. Two of them involve only integrable Hamiltonians ($\lambda = 0$), $\Delta$ being the parameter changed:

(a) $\Delta_I = 0 \rightarrow \Delta_F = 1.5$: from the XX model (non-interacting Hamiltonian) to the XXZ model (interacting Hamiltonian).

(b) $\Delta_I = 1.5 \rightarrow \Delta_F = 0$: from the XXZ model (interacting Hamiltonian) to the XX model (non-interacting Hamiltonian).

The other two quenches have fixed the value of the anisotropy, $\Delta = 0.5$, so that the Hamiltonians are always interacting ones. The quenches involve one strongly chaotic Hamiltonian ($\lambda = 1$) and an integrable one:

(c) $\lambda_I = 1 \rightarrow \lambda_F = 0$: from a chaotic Hamiltonian to the integrable XX model.

(d) $\lambda_I = 0 \rightarrow \lambda_F = 1$: from the XXZ Hamiltonian to a chaotic system.

V. NUMERICAL RESULTS

We analyze a broad range of initial states with energies covering the lower half of the spectrum of the final Hamiltonian. They correspond to eigenstates of $\hat{H}_I$ and are selected according to the value of their energy with respect to $\hat{H}_F$, from very close to the ground state to very close to the middle of the spectrum. For each temperature $T \in [0.1, 100]$ (Boltzmann constant $k_B = 1$), we select the state whose energy $E^{\text{ini}}$ is closest to

$$ E = \frac{1}{Z} \sum \alpha E_\alpha e^{-E_\alpha/T}, \quad (11) $$

where $Z = \sum_\alpha e^{-E_\alpha/T}$ is the partition function. Low temperatures mean energies close to the edge of the spectrum, while high temperatures correspond to energies close to the middle of the spectrum.

We start by studying how the structure of the initial states with respect to $\hat{H}_F$ changes as $T$ increases and then compare it with the results for the observables. To have a quantitative estimate of the proximity between the results from the diagonal ensemble and those from the microcanonical ensemble, we compute their relative difference. For a generic observable $\hat{O}$, this difference is defined by

$$ \delta \hat{O} = \frac{\langle \hat{O} \rangle_{\text{DE}} - \langle \hat{O} \rangle_{\text{ME}}}{\langle \hat{O} \rangle_{\text{DE}}}, \quad (12) $$

To compute the microcanonical averages, we used $\Delta E = 0.4$. We verified that the results were not dependent on this value. Unless indicated, the figures are obtained for $L = 18$ leading to $D = 18 \cdot 564$. Full exact diagonalization is used.

A. Structure of the initial state

In Fig. 1 we compare the distribution of $|C^{\text{ini}}_\alpha|^2$’s as function of the eigenvalues $E_\alpha$ with the energy shell for two temperatures and four quenches. In correspondence with the Gaussian density of states [60], the filling of the shell improves as $T$ increases and the state approaches the middle of the spectrum. In the case of quenches involving two integrable Hamiltonians the improvement is substantial [Figs. 1(a) and (b)]. It is significant also for the quench from an integrable to a chaotic Hamiltonian [Fig. 1(d)], confirming the importance of being away from the edges of the spectrum even when the final Hamiltonian is non-integrable. The least affected state is the one coming from a chaotic Hamiltonian [Fig. 1(c)].

For a more quantitative picture of the filling of the shell, we show in the top panel of Fig. 2 the least square between the distribution of $|C^{\text{ini}}_\alpha|^2$’s and the energy shell. The improvement in the filling of the shell with $T$ is evident for all quenches, but the least square values are overall smaller for the quenches involving a chaotic Hamiltonian and more fluctuating for the quenches between integrable Hamiltonians, especially for XXZ $\rightarrow$ XX. We notice that the constant values of the least squares at very low temperatures (more pronounced for quenches (c) and (d)) is due to the lack of states in that region of the spectrum, so close temperatures lead to the selection of the same initial state.

The middle panel of Fig. 2 shows the value of IPR$^{\text{ini}}$ vs $T$ for the four quenches. It increases with temperature and then saturates. The largest values are reached for the quenches involving a chaotic Hamiltonian, but even in these cases, when $L = 18$, IPR$^{\text{ini}}$ is $\sim 2/3$ of the GOE value $D/3$ (the latter is indicated with a thick dashed line in the figure). For the quenches with two integrable Hamiltonians, IPR$^{\text{ini}}$ is even smaller and large fluctuations are seen, especially for XXZ $\rightarrow$ XX. Therefore, none of the initial states correspond to thermal states at infinite temperature. But more important than the actual value is how IPR$^{\text{ini}}$ scales with system size.
the diagonal entropy \([61]\) with \(E\) and \(E_{\text{ini}}\) is non-mappable to a non-interacting Hamiltonian, since exact diagonalization is required. When comparing the ratio (middle panel) and variance of the energy shell (bottom panel) vs \(T\) for the following quenches: XX \(\rightarrow\) XXZ (green empty diamonds); XXZ \(\rightarrow\) XX (blue empty triangles); (c) chaotic \(\hat{H} \rightarrow\) XXZ (red filled squares); (d) XXZ \(\rightarrow\) chaotic \(\hat{H}\) (black filled circles).

The scaling of \(\text{IPR}^{\text{ini}}\) with \(L\), or equivalently the scaling of the diagonal entropy \([61]\) with \(L\) \([22]\), followed by a comparison with the thermodynamic result, is essential to determining whether thermalization will indeed occur at \(L \rightarrow \infty\). Unfortunately scaling analyses are not possible when \(\hat{H}_F\) is non-mappable to a non-interacting Hamiltonian, since exact diagonalization is required. When comparing the ratio \(\text{IPR}^{\text{ini}}/\text{IPR}_{\text{GOE}}\) vs \(T\) for \(L = 12, 15, 18\), the latter size leads to an overall smoother behavior and possibly larger value for the quenches involving a chaotic Hamiltonian, while large fluctuations remain for the integrable quenches for all system sizes and prevent any general statement [see Fig. 3].

Whether close to the middle of the spectrum, \(\text{IPR}^{\text{ini}}\) grows exponentially with system size for all four quenches or just for some of them is an open question. If it does, then the shell will be better and better filled as \(L\) increases. The width of the energy shell does not surpass that of the density of states, which grows linearly with system size. On the other hand, if the state needs to be too close to the middle of the spectrum, we will be dealing with unrealistically large temperatures. The threshold in energy above which thermalization can happen is also a crucial question that needs to be addressed.

It is informative to look also at the width \(\sigma\) of the energy shell as a function of temperature (bottom panel of Fig. 2). According to Eq. (7), the width of the shell is related to the number of states that are directly coupled with the initial state, that is it quantifies the level of connectivity of the initial state \([32, 53]\). The lowest connectivity is seen for the quench XXZ \(\rightarrow\) XX, which also fluctuates significantly. In contrast, \(\sigma^2\) for the reverse quench, XX \(\rightarrow\) XXZ, reaches the largest values. The smoothest behavior with temperature occurs for
the quench where $\lambda_T = 1$, which leads also to the best filling of the shell and lowest values of least squares.

From the above results, one cannot rule out the possibility of thermalization for the four quenches considered, provided the initial state is away from the edges of the spectrum. One can, however, suspect the quenches involving only two integrable Hamiltonians, especially the case XXZ $\rightarrow$ XX. For this quench, not only do the three quantities in Fig. 2 fluctuate significantly, but scaling analysis in Ref. [22] discourage expectations for thermalization. Interestingly, the reverse case, XX $\rightarrow$ XXZ, fluctuates less in the experimentally accessible region of temperatures in $1 \leq T \leq 10$. The XX and XXZ models are very different, the first having a significantly higher number of degeneracies [35]. Thus, it would not be that surprising if the conclusions for these two quenches at $L \rightarrow \infty$ end up being different.

### B. Local magnetization

The local magnetization, $\hat{S}_i^z$, of each site $i$ is shown in Fig. 4 for the diagonal (circles) and microcanonical (squares) ensembles. For each quench, (a), (b), (c) and (d), the upper panel depicts results for an energy close to the edge of the spectrum ($T = 0.7$), while the lower panel is for an energy close to the middle of the spectrum ($T = 4.0$).

When the temperature is low, the local magnetization shows a strong dependence on the site. This happens for all quenches and is more pronounced at the borders of the chain. As the energy of the initial state approaches the middle of the spectrum, the dependence on the sites almost disappears. A slightly larger value remains on site 1, because of the inclusion of the small defect on the chain [Eq. (10)]. For all quenches at $T = 4.0$, the results for the diagonal ensemble become close to those from the microcanonical ensemble. However, the results are smoother for quenches involving a chaotic Hamiltonian than for those where both Hamiltonians are integrable.

The local magnetization is a good observable for illustrating finite size effects. In the thermodynamic limit, it is irrelevant if the boundaries are periodic or open, all sites should have the same value,

$$\langle \hat{S}_i^z \rangle = -1/6,$$

which is indicated in the figure with a solid line. The fact that we are further from this scenario for quenches (a) and (b) shows how sensitive quenches with only integrable Hamiltonians are to finite system effects. The relative difference [Eq. (12)] for the local magnetization, shown in Fig. 5 indicates that this problem is more evident for quench (b) [XXZ $\rightarrow$ XX]. For each quench in the figure, we choose a site for which the decay of $\delta \hat{S}_i^z$ with temperature is noticeable. For quenches (a), (c) and (d), despite fluctuations, various sites show similar behavior, the infinite time average approaching the thermal result (and the homogeneous -1/6 value) as $T$ increases. For quench (b) the decay for most sites is not visible due to large fluctuations. The site selected is one of the best behaved. Notice also that, when comparing quenches between integrable Hamiltonians with quenches with one chaotic Hamiltonian, $\delta \hat{S}_i^z$ for the latter is approximately one order of magnitude smaller.
C. Spin-spin correlation

The spin-spin correlations between neighboring sites in the middle of the chain is given by

$$C_{L/2,L/2+1}^{\mu\mu} = \langle \hat{S}_{L/2}^\mu \hat{S}_{L/2+1}^\mu \rangle, \quad \mu = x, z. \quad (13)$$

Figure 6 shows the behavior of the longitudinal spin-spin correlation, $C_{L/2,L/2+1}^{zz}$ vs temperature. It approaches the result for an initial thermal state at infinite temperature,

$$C_{L/2,L/2+1}^{zz}(T \to \infty) = \frac{L - 9}{36(L - 1)},$$

but does not equal it, indicating that the initial states considered are not completely extended. The value for $(C_{L/2,L/2+1}^{zz})_{T \to \infty}$ is obtained assuming that the average of $|C_{ini}^{zz}|^2$ is $1/D$, as in the case of eigenstates from full random matrices [6] [see discussion for Eq. 3]. Comparing the results from quenches with two integrable Hamiltonians [Figs. 6 (a) and (b)] with those with one chaotic $\hat{H}$ [Figs. 6 (c) and (d)], we see that the latter are again smoother, especially for the case $\lambda_1 = 0 \to \lambda_F = 1$. For this quench the results are similar also for the correlations between second and third neighbors.

![Graphs showing spin-spin correlations](image)

FIG. 6: (Color online.) Longitudinal spin-spin correlation $C_{L/2,L/2+1}^{zz}$ vs $T$ for the diagonal (black circles) and microcanonical (red squares) ensembles. Quenches as in Fig. 1. The green solid line indicates the result for a thermal state at infinite temperature.

In Fig. 7 we show the absolute value of the difference,

$$\delta_A C_{L/2,L/2+1}^{zz} = \left| (C_{L/2,L/2+1}^{zz})_{DE} - (C_{L/2,L/2+1}^{zz})_{ME} \right|. \quad (14)$$

Since correlations can go to zero, this is a more appropriate quantity than the relative difference. As the initial state approaches the middle of the spectrum, the difference between diagonal and microcanonical averages, despite fluctuating, decreases for all quenches. The values are smaller for the quenches with $\lambda \neq 0$ [Figs. 7(c) and (d)]. In the particular case of XXZ $\to$ chaotic $\hat{H}_F$ [Fig. 7(d)], the decay is slightly perceptible in the region $1 \leq T \leq 10$ and it seems already saturated. The results for $\delta_A C_{L/2,L/2+1}^{zz}$ mirror the filling of the energy shell.

The behavior of $\delta_A C_{L/2,L/2+1}^{xx}$ with temperature is similar to that of $\delta_A C_{L/2,L/2+1}^{zz}$, but the transverse spin-spin correlation vanishes at high temperature.

![Graphs showing absolute difference](image)

FIG. 7: Absolute difference between $(C_{L/2,L/2+1}^{zz})_{DE}$ and $(C_{L/2,L/2+1}^{zz})_{ME}$ vs $T$. Quenches as in Fig. 1.

D. Structure factor

The structure factor, defined as the Fourier transform of the spin-spin correlations [62], corresponds to

$$\hat{S}^{\mu\mu}(k) = \frac{1}{L} \sum_{l,j=1}^L \hat{S}_l^\mu \hat{S}_j^\mu e^{-ik(l-j)}, \quad \mu = x, z. \quad (15)$$

Figure 8 shows results for the diagonal (full symbols) and microcanonical (empty symbols) ensembles for the transverse structure factor $\hat{S}^{zz}(k)$ and two temperatures. The results for $\hat{S}^{zz}(k)$ (not shown) are qualitatively similar, apart from the value for momenta $k = 0, 2\pi$, which is constant and given by $\langle \hat{S}^{zz}(0, 2\pi) \rangle = L/36$ for $S^2 = -L/6$.

As seen in the figure, when the energy of the initial state is close to the edge of the spectrum ($T = 0.7$), both $\langle \hat{S}^{zz}(k) \rangle_{DE}$ and $\langle \hat{S}^{zz}(k) \rangle_{ME}$ have a strong dependence on $k$ for all quenches. This dependence was observed also in Ref. [63], where the initial state was prepared in the ground state of $\hat{H}_I$. When $\hat{H}_F$ has only nearest neighbor couplings, a single peak emerges for $k = \pi$, whereas two peaks exist when second neighbors are included. As $E^{\text{ini}}$ approaches the middle of the spectrum (illustrated for $T = 4.0$), the $k$-dependence...
decreases drastically for all quenches. The results get close, but not equal, to that for a thermal state at infinite temperature, \( \langle \hat{S}_{xx}(k) \rangle_{T \to \infty} = \frac{1}{4} \).

![FIG. 8: (Color online.) Transverse component of the structure factor, \( S_{xx}(k) \). Quenches as in Fig. 1. Two temperatures are shown. Filled symbols are for the diagonal ensemble: \( T = 0.7 \) (green diamonds) and \( T = 4.0 \) (black circles). Empty symbols are for the microcanonical ensemble: \( T = 0.7 \) (blue triangles) and \( T = 4.0 \) (red squares). The green solid line indicates the result for a thermal state at infinite temperature.](image)

In terms of the relative difference [Eq. (12)], the behavior of \( \delta S^{\mu\mu}(k) \) with temperature appears to depend on the direction. In Figs. 9 and 10 we show \( \delta S^{xx}(\pi) \) and \( \delta S^{zz}(\pi) \), respectively. It is not clear if \( \delta S^{xx}(\pi) \) indeed decays with \( T \), even when the quenches involve a chaotic Hamiltonian [Figs. 9(c) and (d)]. But for the latter the values are smaller than for quenches between integrable Hamiltonians [Figs. 9(a) and (b)].

In the \( z \) direction, on the other hand, \( \delta S^{zz}(\pi) \) clearly decreases as the energy of the initial state approaches the middle of the spectrum for quenches with \( \lambda \neq 0 \) [Figs. 10(c) and (d)]. For quenches between integrable Hamiltonians, the decay, if existent, is very subtle.

![FIG. 9: (Color online.) Relative difference for the structure factor in the \( x \) direction vs \( T \). Quenches as in Fig. 1.](image)

![FIG. 10: (Color online.) Relative difference for the structure factor in the \( z \) direction vs \( T \). Quenches as in Fig. 1.](image)

For local magnetization and spin-spin correlations, the proximity between diagonal and microcanonical ensemble decreases with \( T \) for all quenches, but for the structure factor, the picture is less clear. \( \langle \hat{S}_{zz}(\pi) \rangle_{DE} \) approaches \( \langle \hat{S}_{zz}(\pi) \rangle_{ME} \) for quenches involving one chaotic Hamiltonian, while for quenches between two integrable Hamiltonians, only fluctuations are seen. In the \( x \) direction the situation is worse, and the decay of \( \delta S^{xx}(\pi) \) is not evident for any of the quenches. This suggests that non-local observables may be less sensitive to the energy of the initial states than local observables.

In Ref. [21], a study of how the temperature of the initial state affects the properties of the system was also developed. The initial states were thermal (mixed) states evolving accord-

### E. Discussion

As the temperature increases, the results for the observables after relaxation become smoother in position and momentum. They approach the results obtained with thermal states at infinite temperature, but are not equal to them. Therefore, even though the initial states for all quenches get more delocalized as they get closer to the middle of the spectrum, they are not equivalent to the totally delocalized eigenstates from full random matrices.
gathering to a Hamiltonian for hard-core bosons mapped onto non-interacting fermions. Scaling analysis is possible in this case. It was shown that thermalization could only happen for thermal states at infinite temperature. The same may or not be the case when interactions are present, such as for the XXZ model. As we mentioned, the XX and the XXZ models differ significantly in terms of degeneracies [35].

We notice that several works have shown that thermalization does not happen for quenches between two non-interacting integrable Hamiltonians [17, 64–67]. In the present work we have studied quenches between different integrable models or between an integrable and a chaotic Hamiltonian. These scenarios have been much less explored.

VI. CONCLUSIONS

The key factor determining the viability of thermalization in isolated quantum systems is the chaotic structure of the initial state with respect to the Hamiltonian that evolves it. This condition incorporates ETH, since initial states away from the edges of the spectrum fill the energy when the Hamiltonian is chaotic. But it is more general than ETH, because it allows thermalization to occur also when the Hamiltonian is integrable.

Here, we studied how the filling of the energy shell improves as the initial state approaches the middle of the spectrum and how this affects the results for different observables. None of the finite systems considered, where only few-body short-interactions are present, lead to completely extended initial states. Thus, none of them correspond to thermal states at infinite temperature. Nevertheless, they further delocalize as the temperature increases for all quenches, those involving only integrable Hamiltonians: XX → XXZ and XXZ → XX, and those with one chaotic Hamiltonian: XXZ → chaotic model and chaotic Hamiltonian → XXZ.

As the initial state further spreads out with temperature, the results for the observables become smoother. The infinite time averages (diagonal ensemble) approach the thermal averages (microcanonical ensemble). For the structure factors, this approach of ensembles is less evident, apart from \( \delta S^{zz}(\pi) \) when one of the Hamiltonians is chaotic.

Scaling analyses are crucial to resolving whether thermalization can indeed occur for the quenches studied here, but it is not feasible for Hamiltonians non-mappable on non-interacting systems. The only thing that we can see when comparing \( L = 12, 15, \) and \( 18 \), is that fluctuations decrease with system size, especially when one of the Hamiltonians is chaotic. In addition, one needs to determine the threshold in temperature above which thermalization holds and how it depends on the model and system size. If thermalization can occur only for initial states too close to the middle of the spectrum, the temperatures involved are unrealistically large and not of practical use. This may in fact be the case for integrable \( \hat{H}_F \)'s. Alternative methods that do not involve exact diagonalization may be necessary to address these issues.

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