

Absence of thermalization after a local quench and strong violation of the eigenstate thermalization hypothesis

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Absence of thermalization after a *global* quantum quench is a well-established numerical observation in integrable many-body systems, and can be empirically related to a violation of the eigenstate thermalization hypothesis (ETH) in such models. Still, in many of those examples, a weaker version of the conventional ETH (wETH) has been numerically reported or even rigorously proven. In this paper, we show analytically and illustrate numerically that the absence of thermalization is already possible after a *local* quench. A closely related finding is a strong violation of the ETH, meaning that not even the wETH is fulfilled anymore. In our analytical explorations, we focus on XX-spin-chain models with open boundary conditions, where the local quench is generated by initiating the system in thermal equilibrium and then suddenly switching on (or slightly changing) a single-spin impurity either at the end or in the center of the chain. Numerically, we observe qualitatively similar phenomena also for more general XXZ models in the case of an end-impurity, but not in the case of a central impurity.

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I. INTRODUCTION

The problem of thermalization is a long-standing and still not satisfactorily understood issue in statistical physics [1–3]. Essentially, it amounts to the question of why many-body systems can usually be described so successfully by one of the standard canonical ensembles at sufficiently late times, i.e., after the initial relaxation processes have died out.

Considerable new insights have been recently gained by means of the eigenstate thermalization hypothesis (ETH) [4–6], postulating that already the system's energy eigenstates reproduce very accurately its thermal equilibrium properties, at least for generic, so-called nonintegrable models [7]. On the other hand, integrable models are generally expected (or defined) to exhibit an extensive number of conserved quantities in the form of suitable sums of local operators [8]. As a consequence, they are furthermore expected to violate the ETH and hence *not* to thermalize at least after a *global* quantum quench [1,2,7,9], essentially meaning that the initial condition exhibits some nonthermal features throughout the entire system. While there is ample numerical evidence in support of this very appealing general picture, a more rigorous rationale has been provided until now at most in some special cases.

A weaker version of the conventional ETH (wETH) proposes that the system's thermal equilibrium properties are well captured by the vast majority of its energy eigenstates, but still admits some sufficiently small fraction of exceptions [10]. In

contrast to the conventional (or “strong”) ETH, the wETH can even be rigorously proven for a large class of Hamiltonians, the main prerequisites being that the system is translationally invariant and exhibits only short-range interactions, while the issue of integrability does not seem to play any role. Furthermore, such systems have been analytically shown to exhibit (re)thermalization after a *local* quantum quench, for instance, in Refs. [11–13], and it has been argued that such a behavior should be expected to occur very generally [14,15].

The main message of our present paper is that things are actually more subtle. Namely, we will provide analytical examples exhibiting the absence of thermalization after a local quench, accompanied by a violation even of the wETH, which we dub a *strong violation of the ETH*. Note that this does not contradict the above mentioned previous findings since our present examples are *not* translationally invariant. It also does not contradict the numerical observation of thermalization after a local quench, for instance, in Refs. [14,16–20]. The reason is that in those latter examples the local quench breaks the integrability of the system, but not in our present examples.

Specifically, we will analytically explore the XX-spin-chain model with open boundary conditions after switching-on (or slightly changing) an impurity either at the chain-end or in the middle of the chain. Furthermore, we will numerically demonstrate that also the more general XXZ model behaves qualitatively similarly for impurities at the chain-end, but very differently for central impurities.

The rest of the paper is organized as follows. In Sec. II, we provide the details of the considered spin-chain models and local quenches, the notions of (non)thermalization and strong violation of the ETH, and how they can be related to temporal correlations at thermal equilibrium. In Secs. III and IV, we analytically explore and numerically illustrate for the

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XX model with an end-impurity those correlations and their implications regarding the issues of (non)thermalization and strong violation of the ETH. In Sec. V, the same properties for the XXZ model are recovered by numerical means. In Sec. VI, we provide similar analytical and numerical explorations, but now for the case of a central- instead of an end-impurity, and resulting in a very different behavior of the XX and the XXZ models with respect to (non)thermalization and the ETH.

II. GENERAL FRAMEWORK

A. Setup

Our starting point is the spin-1/2 XXZ-chain Hamiltonian with open boundary conditions:

$$H_{\text{XXZ}} = \sum_{l=1}^{L-1} J_{\perp} (s_{l+1}^x s_l^x + s_{l+1}^y s_l^y) + J_z s_{l+1}^z s_l^z, \quad (1)$$

where the s_l^a with $a \in \{x, y, z\}$ are spin-1/2 operators at the chain sites $l \in \{1, \dots, L\}$ and the coupling parameters $J_{\perp}$ and J_z quantify the nearest neighbor interactions [21].

Upon adding a single magnetic impurity at an arbitrary but fixed chain site $v \in \{1, \dots, L\}$, we obtain the modified Hamiltonian

$$H_0 = H_{\text{XXZ}} + \gamma s_v^z, \quad (2)$$

where γ may be viewed as a localized transverse field. In the first part of the paper (Secs. III and IV), we will focus on the special case $J_{\perp} = 1$ and $J_z = 0$ (XX model). In the second part of the paper and in the rest of the present section, we will deal with the more general XXZ model.

The initial state of the system is assumed to be given by a canonical ensemble (Gibbs state) associated with H_0 from Eq. (2),

$$\rho(0) := e^{-\beta H_0} / \text{tr}\{e^{-\beta H_0}\}, \quad (3)$$

$$\beta := 1/k_B T, \quad (4)$$

where T is the temperature and k_B Boltzmann's constant.

The temporal evolution of this initial state is governed by a perturbed Hamiltonian of the form

$$H = H_0 + gV, \quad (5)$$

with a local perturbation operator V and a coupling parameter g . Working in units with $\hbar = 1$, the system's state at time $t > 0$ can thus be written as

$$\rho(t) = e^{-iHt} \rho(0) e^{iHt}, \quad (6)$$

and the concomitant expectation value of an observable A (Hermitian operator) as

$$\langle A \rangle_t := \text{tr}\{\rho(t)A\}. \quad (7)$$

For generic perturbations in Eq. (5), the Hamiltonian H , which governs the dynamics, is different from H_0 and the Gibbs state (3) amounts to a nonequilibrium initial condition. Put differently, the system is in thermal equilibrium with respect to the Hamiltonian H_0 for all times $t < 0$, experiences an instantaneous parameter change at $t = 0$ (quantum quench) and is governed by H for $t > 0$.

Throughout our present work, we will focus on perturbations which are identical to the impurity in Eq. (2), i.e.,

$$V = s_v^z. \quad (8)$$

Of particular interest are cases with $\gamma = 0$ in Eq. (2), meaning that an impurity is suddenly “switched-on” at $t = 0$. More generally, i.e., for $\gamma \neq 0$, the impurity is already present at times $t < 0$, and suddenly changes its strength at $t = 0$. We also remark that generalizations to different spins in Eqs. (2) and (8), say s_{μ}^z instead of s_v^z in Eq. (8), would, in principle, be straightforward, but technically much more involved, and, moreover, seem to us of relatively minor physical interest.

B. Thermalization and sufficient conditions for nonthermalization

At the focus of our present work is the issue of (non)thermalization, i.e., the question of whether or not the expectation values in Eq. (7) approach for sufficiently large chain-lengths L and after sufficiently long times t their thermal equilibrium value

$$\langle A \rangle_{\text{th}} := \text{tr}\{\rho_{\text{can}} A\}, \quad (9)$$

where ρ_{can} is the canonical ensemble

$$\rho_{\text{can}} := e^{-\beta H} / \text{tr}\{e^{-\beta H}\} \quad (10)$$

pertaining to the postquench Hamiltonian H , see also Eqs. (5) and (6).

The following four remarks will be of considerable importance later on. (i) Note that we tacitly have chosen the same β in Eqs. (3) and (10). The intuitive justification is that a local perturbation [see Eqs. (5) and (8)] should not notably change the temperature for sufficiently large systems. A more detailed and rigorous justification is provided in Appendix A. (ii) Since our models amount to isolated systems, it might appear more natural to work with a microcanonical instead of a canonical ensemble in Eq. (9). We tacitly take for granted that both ensembles would result in (practically) identical thermal expectation values at least for those Hamiltonians and observables we will consider in the following. A more rigorous justification of this equivalence of ensembles is provided, for instance, in Refs. [22–25]. Analogous remarks apply to the initial condition in Eq. (3). (iii) Usually, the expectation values in Eq. (7) are notably different from the thermal value in Eq. (9) during some initial time-interval (relaxation process), but also at certain, arbitrarily large times t (quantum recurrences or revivals). With increasing system size, those exceptional times are furthermore expected to become more and more rare. In other words, a necessary (but possibly not sufficient) condition for thermalization is that the long-time average of the expectation values in Eq. (7) approaches the thermal value in Eq. (9) as the system size increases. In the following, we will be mainly interested in examples, which do *not* exhibit thermalization. Accordingly, we will utilize as a sufficient condition for nonthermalization the criterion that the difference between the long-time average and the thermal value remains finite for arbitrarily large system sizes (thermodynamic limit). (iv) In order to demonstrate nonthermalization, it is furthermore sufficient that this criterion is fulfilled at least for one physically relevant observable A . With

respect to our specific model from Eq. (5), we will therefore mainly focus on particularly simple observables of the form

$$A = s_\alpha^z, \quad (11)$$

where $\alpha \in \{1, \dots, L\}$ may be different or equal to the index ν of the perturbation V in Eq. (8).

C. The role of the temporal correlations

Exploiting Eq. (6) and the cyclic invariance of the trace, the expectation values in Eq. (7) can be rewritten as

$$\langle A \rangle_t = \text{tr}\{\rho(0)A(t)\}, \quad (12)$$

where

$$A(t) := e^{iHt} A e^{-iHt} \quad (13)$$

is the observable at time t in the Heisenberg picture. Similarly, the temporal correlation (also called, among others, dynamic or two-point correlation function) of two Hermitian operators V and A at thermal equilibrium is defined as

$$C_{VA}(t) := \langle VA(t) \rangle_{\text{th}} - \langle V \rangle_{\text{th}} \langle A \rangle_{\text{th}}. \quad (14)$$

While V and A in this definition are still arbitrary, for our present purposes it is sufficient to focus on the situation that V is the local perturbation from Eq. (5) and A some local observable, as exemplified by Eqs. (8) and (11), respectively. The reason is that in this way it becomes possible to utilize the generalization of Onsager's regression hypothesis from Ref. [26], consisting in the approximation [27]

$$\langle A \rangle_t - \langle A \rangle_{\text{th}} = g\beta \tilde{C}_{VA}(t), \quad (15)$$

$$\tilde{C}_{VA}(t) := \sum_{k=0}^{\infty} \frac{(i\beta)^k}{(k+1)!} \frac{d^k}{dt^k} C_{VA}(t). \quad (16)$$

Note that the correlations in Eq. (14) are generally complex-valued, and likewise for every single summand on the right-hand side of Eq. (16), while the entire sum is provably real-valued [26].

Roughly speaking, the relative error of the approximation (15) becomes arbitrarily small for sufficiently small values of $g\beta$. More precisely speaking, the neglected terms can be rigorously shown [26] to be upper bounded (in modulus) by $g^2\beta^2 \|V\|_{\text{op}}^2 \|A\|_{\text{op}} q(\beta)$, where $\|V\|_{\text{op}}$ is the operator norm of V (largest eigenvalue in modulus) and thus $\|V\|_{\text{op}} = \|A\|_{\text{op}} = 1/2$ for our standard examples from Eqs. (8) and (11) (see also Ref. [21]). Furthermore, the function $q(\beta)$ is of order unity at least for small-to-moderate values of $\beta J_\perp$, βJ_z , and $\beta(g + \gamma)$ in the case of our Hamiltonians (5) of the specific form (1), (2), and (8).

These general analytical predictions regarding the accuracy of the approximation (15) have been numerically confirmed by a wide variety of examples in Refs. [13,26]. A few more such example will also be presented later. For the rest, our present mindset and foremost objective will be different: Taking the relation (15) for granted, we will deduce from it without any further approximation that certain models of the form (1)–(8) do *not* exhibit thermalization after a local (and sufficiently weak) quantum quench.

From Eqs. (2) and (8), it follows that the Hamiltonian H in Eq. (5) does not depend separately on γ and g , but only on the

combination

$$p := 2(g + \gamma), \quad (17)$$

where the extra factor 2 has been introduced for later convenience. The same property is inherited via Eq. (10) by the thermal equilibrium values in Eq. (9), the correlations in Eq. (14), and the quantity $\tilde{C}_{VA}(t)$ in Eq. (16). Moreover, for observables of the specific form (11), it has been shown in Ref. [28] (see Supplemental Material I.D therein) that the thermal equilibrium values in Eq. (9) are odd functions of p , while the correlations in Eq. (14) are even functions of p . It follows that also the quantity $\tilde{C}_{VA}(t)$ in Eq. (16) must be an even function of p , i.e., invariant under a sign change of p . For the correlations in Eq. (14) and the quantity $\tilde{C}_{VA}(t)$ in Eq. (16), exactly the same invariance can be shown to apply under a sign change of the coupling parameter $J_\perp$ in Eq. (1). Moreover, the same symmetry properties can be extended to arbitrary observables of the form $A = s_i^a$. Analogous generalizations are also valid for the modulus of the thermal equilibrium values in Eq. (9), while the behavior of the sign is more complicated [28].

D. Nonthermalization and strong violation of the ETH

Let us define the long-time average of an arbitrary function $f(t)$ as

$$\overline{f(t)} := \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt f(t). \quad (18)$$

Under very weak assumptions regarding the long-time behavior of $C_{VA}(t)$, which we henceforth tacitly take for granted, it readily follows that the long-time average of $d^k C_{VA}(t)/dt^k$ is zero for any $k \geq 1$. We thus can conclude from Eq. (16) that

$$\overline{\tilde{C}_{VA}(t)} = \overline{C_{VA}(t)}. \quad (19)$$

According to items (iii) and (iv) above Eq. (11), the difference on the left-hand side of Eq. (15) plays a key role with respect to the question of (non)thermalization: a sufficient condition for nonthermalization is a nonvanishing long-time average of this difference in the thermodynamic limit, which in turn can be written by means of Eqs. (15) and (19) as

$$\overline{\langle A \rangle_t - \langle A \rangle_{\text{th}}} = g\beta \overline{C_{VA}(t)}. \quad (20)$$

In other words, a nonvanishing value of $\overline{C_{VA}(t)}$ for at least one local observable A implies nonthermalization [and given this approximation itself is sufficiently accurate, as discussed below Eq. (16)].

Denoting by $\mathcal{E}_n$ and $|n\rangle$ the eigenvalues and eigenvectors of the Hamiltonian H , choosing $V = A$, and exploiting Eqs. (9) and (14)–(19), one can readily show [28–30] that

$$\langle A \rangle_{\text{th}} = \sum_{n=1}^N p_n \langle n|A|n \rangle, \quad (21)$$

$$\overline{C_{AA}(t)} = \sum_{n=1}^N p_n [\langle n|A|n \rangle - \langle A \rangle_{\text{th}}]^2, \quad (22)$$

where $p_n := \langle n|\rho_{\text{can}}|n \rangle = e^{-\beta \mathcal{E}_n} / \sum_{m=1}^N e^{-\beta \mathcal{E}_m}$ is the population of the energy level $|n\rangle$ in the canonical ensemble from

Eq. (11), and where—in case that H exhibits degeneracies—the eigenstates $|n\rangle$ must be chosen so that A is diagonal in the corresponding eigenspaces of H .

Taking for granted the equivalence of ensembles [see also items (ii) above Eq. (11)], a non-negligible value of the sum in Eq. (22) is thus readily found [30] to be tantamount to a violation of the wETH as defined in Refs. [10], and thus to a strong violation of the ETH, see also Secs. I and IV D. According to the discussion below Eq. (20), both properties furthermore imply the absence of thermalization after a *local* quench. Note that this is similar but different from the well-established (mainly numerical) finding that a violation of the conventional (strong) ETH implies nonthermalization after a *global* quench [7].

We close with two noteworthy remarks. (i) Sections II B–II D and, in particular, the conclusions in the previous paragraph, are not restricted to the specific XXZ model from Eqs. (1), (2), and (5), which we consider in the rest of the paper, but are valid more generally. (ii) To prove the occurrence instead of the absence of thermalization after a local quantum quench, it is *not* sufficient to show that Eq. (22) approaches zero in the thermodynamic limit. Instead, one has to show that the time-average on the right-hand side of Eq. (20) approaches zero for *all* local observables A [and the given perturbation V under consideration in Eq. (5)]. Moreover, it is not sufficient to show that the time-average $\overline{\langle A \rangle}_t$ on the left-hand side of Eq. (20) approaches the thermal value $\langle A \rangle_{\text{th}}$. Instead, one has to show that the time-dependent deviations $\langle A \rangle_t - \langle A \rangle_{\text{th}}$ become negligibly small for all (sufficiently late) times t [apart from negligibly rare exceptions (quantum revivals), see also item (iii) below Eq. (10)]. A more detailed investigation of this issue has been carried out in Ref. [13].

III. THE XX MODEL

The XX model amounts to a special case of Eq. (1) with parameters

$$J_{\perp} = 1, \quad J_z = 0. \quad (23)$$

Exploiting Eqs. (1), (2), (8), and (17), the Hamiltonian (5) thus assumes the form [21]

$$H = \sum_{l=1}^{L-1} (s_{l+1}^x s_l^x + s_{l+1}^y s_l^y) + \frac{p}{2} s_v^z. \quad (24)$$

A. Jordan-Wigner transformation

It is well-known that the Hamiltonian (24) can be analytically diagonalized by mapping it via a Jordan-Wigner transformation to an equivalent model of free (noninteracting, spinless) fermions, and is therefore often denoted as a noninteracting integrable model [31]. For a very incomplete selection of pertinent previous works, employing these well-established concepts to similar models as in our present paper, we refer to Refs. [9,32–36] and further references therein. Accordingly, we confine ourselves to a very brief summary of the main steps, the full details of which can be found, for instance, in Ref. [13]. In a first step, the raising and lowering Pauli matrices $\sigma_l^{\pm} := \sigma_l^x \pm i\sigma_l^y$ are employed to define the

operators

$$c_l := \sigma_l^- Z_l, \quad Z_l := \prod_{k=1}^{l-1} (-\sigma_k^z), \quad (25)$$

and their adjoint counterparts $c_l^{\dagger}$, which are then shown to fulfill the anti-commutation relations characteristic of fermionic annihilation and creation operators. Moreover, Eq. (24) can be rewritten [21] as

$$H = \frac{1}{2} \sum_{l=1}^{L-1} (c_{l+1}^{\dagger} c_l + c_l^{\dagger} c_{l+1}) + \frac{p}{2} c_v^{\dagger} c_v \quad (26)$$

apart from an irrelevant additive constant. The second step is based on the observation that for any given unitary $L \times L$ matrix U with matrix elements U_{kl} , the operators

$$f_k := \sum_{l=1}^L U_{kl} c_l \quad (27)$$

and their adjoint counterparts $f_k^{\dagger}$ are again fermionic annihilation and creation operators. Moreover, by suitably choosing the unitary U , the correspondingly transformed Hamiltonian from Eq. (26) assumes the form

$$H = \sum_{k=1}^L E_k f_k^{\dagger} f_k \quad (28)$$

with real valued energies E_k [not to be confused with the energies $\mathcal{E}_n$ above Eq. (21)]. As shown in Appendix A of Ref. [13], for our specific example from Eq. (24) the matrix elements U_{kl} of this unitary U and the energies E_k must solve, for any given $k \in \{1, \dots, L\}$, the L coupled linear equations

$$U_{kl+1}^* \bar{\delta}_{lL} + U_{kl-1}^* \bar{\delta}_{l1} = (2E_k - p \delta_{lv}) U_{kl}^*, \quad (29)$$

where l runs from 1 to L , δ_{jk} is the Kronecker delta, and $\bar{\delta}_{jk} := 1 - \delta_{jk}$.

Let us abbreviate by $|0\rangle := |\downarrow \dots \downarrow\rangle$ the specific L -spin product state where every single spin is in the “down” state in the eigenbasis of s_l^z , i.e. [21], $\sigma_l^z |0\rangle = -|0\rangle$ for any $l \in \{1, \dots, L\}$. It follows that $\sigma_l^- |0\rangle = 0$, hence $c_l |0\rangle = 0$, and finally $f_l |0\rangle = 0$ for all $l \in \{1, \dots, L\}$. In other words, $|0\rangle$ plays the role of the vacuum state with respect to the fermionic models in Eqs. (26) and (28).

Denoting by $\vec{b} := (b_1, \dots, b_L)$ a vector with L “binary” components $b_k \in \{0, 1\}$, we define

$$|\vec{b}\rangle := (f_1^{\dagger})^{b_1} (f_2^{\dagger})^{b_2} \dots (f_L^{\dagger})^{b_L} |0\rangle. \quad (30)$$

One thus can infer from Eq. (28) that

$$H |\vec{b}\rangle = E(\vec{b}) |\vec{b}\rangle, \quad (31)$$

$$E(\vec{b}) := \sum_{k=1}^L b_k E_k. \quad (32)$$

In other words, the 2^L different vectors $|\vec{b}\rangle$ are the eigenstates of H and $E(\vec{b})$ the corresponding eigenvalues. [Hence, there must exist a one-to-one relation to the eigenvectors $|n\rangle$ and eigenvalues $\mathcal{E}_n$ introduced above Eq. (21), apart from some complications which possibly may arise in the case

of degeneracies, see below Eq. (22).] Finally, in order to evaluate Eq. (14), the above Jordan-Wigner and unitary transformations must also be applied to the perturbations V and observables A of interest. For our particular examples from Eqs. (8) and (11), one thus may exploit Eq. (25) to infer [13] the relation

$$s_l^z = c_l^\dagger c_l - 1/2. \quad (33)$$

Finally, $c_l^\dagger c_l$ on the right-hand side of Eq. (33) must be expressed in terms of the operators f_k and $f_k^\dagger$ via the inversion of Eq. (27), i.e.,

$$c_l = \sum_{k=1}^L U_{kl}^* f_k, \quad (34)$$

and likewise for $c_l^\dagger$.

B. Previous results and remaining task

By means of this formalism, it is possible to evaluate the temporal correlations in Eq. (14) as well as the infinite sum on the right-hand side of Eq. (16) in closed analytical form without any further approximation. Referring to Ref. [13] for the detailed calculations, the so-obtained result for Eq. (16) can be written in the form

$$\tilde{C}_{VA}(t) = \sum_{j,k=1}^L U_{jv} U_{j\alpha}^* U_{kv}^* U_{k\alpha} f_{jk} e_{jk}(t), \quad (35)$$

$$f_{jk} := \frac{\tanh(\beta E_j/2) - \tanh(\beta E_k/2)}{2\beta(E_j - E_k)}, \quad (36)$$

$$e_{jk}(t) := e^{-i(E_j - E_k)t}. \quad (37)$$

It immediately follows that Eq. (36) and thus (35) are even functions of β . By interchanging the summation indices j and k one furthermore sees that the right-hand side of Eq. (35) is equal to its complex conjugate, i.e., we recover the general prediction below Eq. (16) that $\tilde{C}_{VA}(t)$ must be a real-valued function of t .

The remaining task is the explicit solution of Eq. (29). To simplify the notation, let us temporarily consider $k \in \{1, \dots, L\}$ as arbitrary but fixed, and employ the abbreviations

$$E := E_k, \quad (38)$$

$$a_l := \kappa U_{kl}^*. \quad (39)$$

Moreover, while the U_{kl} are normalized according to $\sum_l |U_{kl}|^2 = 1$, we do not require such a normalization condition for the a_l 's. This is accounted for by the still arbitrary proportionality constant $\kappa \in \mathbb{C}$ in Eq. (39). Our only requirement is that $\kappa \neq 0$, or equivalently, that at least one of the a_l 's must be nonzero. Adopting these abbreviations, Eq. (29) amounts to

$$\bar{\delta}_{Ll} a_{l+1} + p \delta_{vl} a_l + \bar{\delta}_{1l} a_{l-1} = 2E a_l, \quad (40)$$

where l runs from 1 to L .

It is instructive to rewrite those L equations in the form $K\vec{a} = E\vec{a}$, where $\vec{a}$ is a L -dimensional column vector with components a_l , and K is a $L \times L$ matrix with elements $K_{ml} :=$

$[\delta_{l+1m} + p\delta_{vl}\delta_{lm} + \delta_{l-1m}]/2$. Observing that $K_{ml} = K_{lm}$ it follows that K is self-adjoint, i.e., we are actually dealing with a Hermitian matrix eigenvalue problem. Moreover, we can conclude from Eqs. (38) and (39) that the eigenvector $\vec{a}$ with eigenvalue $E = E_k$ can be identified (up to normalization) with the k -th column vector of the unitary matrix $U^\dagger$.

Altogether, we are thus left with the task to determine the L solutions of the eigenvalue problem (40). The energies E_k and matrix elements U_{kl} then readily follow as detailed in and around Eqs. (38) and (39).

Before doing so, some general properties of those solutions are noteworthy. To begin with, we note that for any given solution a_l of Eq. (40), also the real and imaginary parts of a_l will be solutions. It follows that, if it is convenient, we always may assume without loss of generality that the a_l and hence the U_{kl} in Eq. (39) are purely real quantities. We thus can infer that Eq. (35) is symmetric with respect to the indices v and α , and hence with respect to the perturbation V in Eq. (8) and the observable A in Eq. (11). Moreover, one sees that a sign change of t is tantamount to a complex conjugation of Eq. (35). Recalling that Eq. (35) is real-valued [see below Eq. (37)], the result is an invariance under time-inversion. Finally, given any solution of Eq. (40), let us define $p' := -p$, $E' := -E$, and $a'_l := (-1)^l a_l$. It readily follows from Eq. (40) that

$$\bar{\delta}_{Ll} a'_{l+1} + p' \delta_{vl} a'_l + \bar{\delta}_{1l} a'_{l-1} = 2E' a'_l. \quad (41)$$

In other words, for every solution of the original problem, we found a solution with an inverted sign of p . Together with the discussion around Eqs. (38) and (39) one thus can conclude that a sign change of p implies a sign change of the energies E_k (possibly after some suitable permutation of the labels k), and that each matrix element U_{kl} acquires a factor $(-1)^l$. Moreover, one can conclude that a sign change of p is tantamount to interchanging the summation indices j and k on the right-hand side of Eq. (35). Recalling the discussion below Eq. (37) it follows that the sum is invariant under a sign change of p , i.e., we recover the general prediction below Eq. (17) that $\tilde{C}_{VA}(t)$ must be an even function of p .

IV. THE XX-MODEL WITH AN END-IMPURITY

We focus on impurities and perturbations s_v^z in Eqs. (2) and (8) [and thus in Eq. (24)] with

$$v = L, \quad (42)$$

i.e., we may imagine the impurity to be located at the right chain-end [see also discussion below Eq. (8)]. Accordingly, the L equations (40) can be rewritten as

$$a_{l+1} + a_{l-1} = 2E a_l \quad \text{for } l = 2, \dots, L-1, \quad (43)$$

$$a_2 = 2E a_1, \quad (44)$$

$$a_{L-1} + p a_L = 2E a_L. \quad (45)$$

A systematic solution of these equations is still very difficult. Hence, we will start out from an ansatz with some free parameter, and then show that it solves Eqs. (43)–(45) by suitably choosing the parameter. Moreover, we will show that the ansatz indeed generates L different such solutions

[see below Eq. (40)]. In other words, a complete solution of the original problem is obtained, thus, justifying the ansatz *a posteriori*.

A. Ansatz

Our starting point is the observation that the quantities

$$\alpha_l := \sin(\varphi l) \quad \text{for all } l \in \mathbb{Z} \quad (46)$$

satisfy for an arbitrary but fixed $\varphi \in \mathbb{C}$, the relations

$$\alpha_{l+1} + \alpha_{l-1} = 2 \cos(\varphi) \alpha_l \quad \text{for all } l \in \mathbb{Z}. \quad (47)$$

In view of Eq. (43), this observation suggests the ansatz

$$E = \cos(\varphi), \quad (48)$$

$$a_l = \alpha_l = \sin(\varphi l) \quad \text{for } l = 1, \dots, L, \quad (49)$$

with a generally *complex valued* parameter φ . By exploiting Eqs. (46) and (47), one readily verifies that this ansatz indeed solves not only Eq. (43) but also Eq. (44). We are thus left to solve the remaining equation (45) by suitably choosing the parameter $\varphi \in \mathbb{C}$. In fact, we have to show that there exist L different solutions of this equation (see above).

Introducing Eq. (49) into Eq. (45) yields

$$2E a_L - p \alpha_L = \alpha_{L-1} = 2E \alpha_L - \alpha_{L+1}, \quad (50)$$

where we exploited Eqs. (47) and (48) in the last step. It follows that $p \alpha_L = \alpha_{L+1}$ and with Eq. (46) that

$$\sin(\varphi(L+1)) = p \sin(\varphi L). \quad (51)$$

Altogether, considering the quantities L and p as given, we are left to determine L solutions $\varphi \in \mathbb{C}$ of Eq. (51). More precisely speaking, we are actually not interested in the solutions φ of Eq. (51) themselves, but rather in the concomitant eigenvectors and eigenvalues, encoded by $\{a_l\}_{l=1}^L$ and E , which derive from φ via Eqs. (48) and (49). For instance, one readily sees that φ and $\varphi + 2\pi$ give rise via Eqs. (48) and (49) to exactly the same eigenvectors and eigenvalues, hence we can and will restrict ourselves to φ 's with the property $\text{Re}(\varphi) \in (-\pi, \pi]$. Likewise, φ gives rise via Eqs. (48) and (49) to the same eigenvectors and eigenvalues as $-\varphi$ [apart from an irrelevant sign change of all a_l , see below Eq. (39)]. Accordingly, we can and will restrict ourselves to φ 's which satisfy the extra condition

$$\text{Re}(\varphi) \in [0, \pi]. \quad (52)$$

Finally, in the special cases $\varphi = 0$ and $\varphi = \pi$ it follows from Eq. (49) that $a_l = 0$ for all $l = 1, \dots, L$, which we excluded below Eq. (39). Hence, Eq. (52) must be complemented by the additional constraint

$$\varphi \notin \{0, \pi\}. \quad (53)$$

As mentioned below Eq. (28) (see also below Eq. (40)), only real eigenvalues E are admissible in Eq. (38). Writing φ as $x + iy$ with $x, y \in \mathbb{R}$, one readily sees that the right-hand side of Eq. (48) is real if and only if $\sin(x) \sinh(y) = 0$, which in turn is only possible in one of the following two cases.

Case A: $\sinh(y) = 0$ with $y \in \mathbb{R}$, implying $y = 0$, and thus $\varphi \in \mathbb{R}$. Together with Eqs. (52) and (53), this amounts

to the requirement

$$\text{case A: } \varphi \in (0, \pi). \quad (54)$$

Case B: $\sin(x) = 0$ with $x \in \mathbb{R}$, implying $x/\pi \in \mathbb{Z}$ and thus $\varphi = iy + n\pi$ with $y \in \mathbb{R}$ and $n \in \mathbb{Z}$. Similarly as above Eq. (52), one sees that it is actually sufficient to focus on $y \in \mathbb{R}_0^+$ and $n \in \{0, 1\}$. Together with Eqs. (52) and (53), this amounts to the requirement

$$\text{case B: } \varphi = iy + n\pi \quad \text{with } y \in \mathbb{R}^+ \text{ and } n \in \{0, 1\}. \quad (55)$$

In the latter case B, it is for practical purposes more convenient to replace φ in Eq. (49) by $i\varphi$, yielding (apart from an irrelevant factor i , see below Eq. (39))

$$a_l = \sinh(\varphi l) \quad \text{for } l = 1, \dots, L. \quad (56)$$

Similarly, Eqs. (48) and (51) now assume the form

$$E = \cosh(\varphi), \quad (57)$$

$$\sinh(\varphi(L+1)) = p \sinh(\varphi L). \quad (58)$$

Observing that above Eq. (55) we could equivalently replace the condition $y \in \mathbb{R}_0^+$ by the condition $y \in \mathbb{R}_0^-$, the requirement (55) now assumes the form

$$\text{case B: } \varphi = y + in\pi \quad \text{with } y \in \mathbb{R}^+ \text{ and } n \in \{0, 1\}. \quad (59)$$

B. Analytical solution

In this section, we work out the details of the ansatz from the previous Sec. IV A. In particular, we will treat the two cases in and above Eqs. (54) and (59) in two separate sections. A summary and discussion of the so obtained solutions is provided in the subsequent Sec. IV C, including the notions of (de)localized modes appearing in the titles of the next sections.

1. Case A: delocalized modes

According to Eqs. (51) and (54), we have to solve

$$\sin(\varphi(L+1)) = p \sin(\varphi L) \quad \text{with } \varphi \in (0, \pi). \quad (60)$$

To begin with, we show that there exists no solution of (60) with the property $\sin(\varphi L) = 0$ by means of a proof by contradiction. Let us therefore assume that there exists a solution with $\sin(\varphi L) = 0$. The condition $\varphi \in (0, \pi)$ in Eq. (60) implies that $\varphi L = \pi n$ with $n \in \{1, \dots, L-1\}$. Similarly, we can conclude from Eq. (60) that $\sin(\varphi(L+1)) = 0$, and thus $\varphi(L+1) = \pi m$ with $m \in \{1, \dots, L\}$. In other words, we are looking for solutions of the equation $L/(L+1) = n/m$ with $n \in \{1, \dots, L-1\}$ and $m \in \{1, \dots, L\}$. One readily sees that no such solution exists: Observing that n must be smaller than L and smaller than m , it follows that $n/m \leq n/(n+1) < L/(L+1)$.

Accordingly, we can and will focus on $\sin(\varphi L) \neq 0$ in Eq. (60), and our goal is to find solutions of

$$f(\varphi) = p \quad \text{with } \varphi \in (0, \pi), \quad (61)$$

$$\begin{aligned} f(x) &:= \frac{\sin(x(L+1))}{\sin(xL)} \\ &= \cos(x) + \sin(x) \cot(xL), \end{aligned} \quad (62)$$

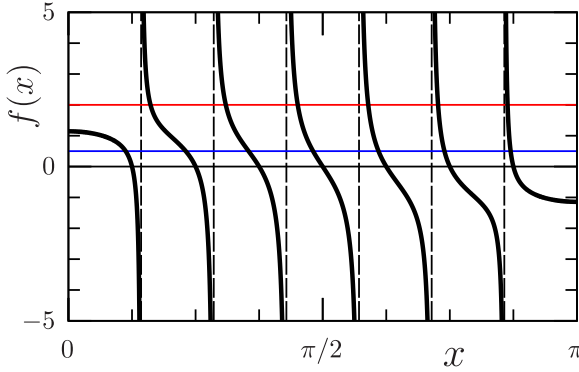


FIG. 1. Black: the function $f(x)$ from Eq. (62) for $L = 7$ and $x \in (0, \pi)$ [see Eq. (61)]. The dashed vertical lines are meant to indicate the $L - 1$ poles of $f(x)$. The intersections of the black curve with the red horizontal line exemplify the graphical solutions of Eq. (61) when choosing $p = 2$. Obviously, there are $L - 1$ intersections. Likewise, the intersections with the blue line exemplify the L solutions when $p = 0.5$.

where we exploited that $\sin(x(L + 1)) = \sin(xL)\cos(x) + \cos(xL)\sin(x)$ in the last step.

Next we turn to a closer inspection of the function $f(x)$ from Eq. (62) with $x \in (0, \pi)$ [see Eq. (61)]. An illustration for $L = 7$ is provided in Fig. 1. The following main properties of $f(x)$ can be readily verified analytically or by looking at Fig. 1. (i) It exhibits the symmetry $f(\pi - x) = -f(x)$ [37]. (ii) It exhibits L zeros at $x = n\pi/(L + 1)$ with $n \in \{1, \dots, L\}$. (iii) It exhibits $L - 1$ simple poles at $x = m\pi/L$ with $m \in \{1, \dots, L - 1\}$, and is strictly monotonically decreasing for all other $x \in (0, \pi)$ (the analytical proof is provided in Appendix B). (iv) It approaches the value

$$p_c := \frac{L + 1}{L} \quad (63)$$

for $x \rightarrow 0$ and the value $-p_c$ for $x \rightarrow \pi$. With these properties of $f(x)$ in mind, we are in the position to discuss the solutions of Eq. (61).

Let us first focus on the case $|p| > p_c$. From the properties (iii) and (iv) or from Fig. 1, one can conclude that every pole of $f(x)$ gives rise to exactly one solution of Eq. (61). Furthermore, each solution is a strictly monotonically decreasing function of p . Finally, the distance of every given solution to the corresponding pole has the same sign as p and cannot exceed the distance between neighboring poles. In other words, there are $L - 1$ pairwise distinct solutions of Eq. (61) of the form

$$\varphi_k = \frac{\pi k + r_k}{L} \quad \text{with } k \in \{1, \dots, L - 1\}, \quad (64)$$

where the “remainders” r_k exhibit the same sign as p , are strictly monotonically decreasing functions of p , and are bounded according to

$$|r_k| < \pi. \quad (65)$$

Finally, by combining Eq. (64) with Eqs. (38), (39), (48), and (49), we obtain

$$E_k = \cos\left(\frac{\pi k + r_k}{L}\right), \quad (66)$$

$$U_{kl} = \kappa_k^{-1} \sin\left(\frac{l\pi k + lr_k}{L}\right), \quad (67)$$

for $k \in \{1, \dots, L - 1\}$ and $l \in \{1, \dots, L\}$, where

$$\kappa_k := \left(\sum_{l=1}^L \sin^2\left(\frac{l\pi k + lr_k}{L}\right)\right)^{1/2} \quad (68)$$

is a normalization constant.

Our next observation is that $f(x)$ in Eq. (62) can be approximated by $1 + x \cot(xL)$ for small x . For large L , this implies that $f(x)$ stays very close to unity with the exception of a very small neighborhood of all those poles which are located near zero. We thus can conclude that $|r_k| \ll \pi$ for all $k \ll L$. [This can *not* be seen in Fig. 1 since the value of $L = 7$ is still too small.] Analogous conclusions apply for x close to π and thus for all k with $L - k \ll L$. Finally, it is obvious from Fig. 1 that all r_k approach zero for asymptotically large $|p|$. In all the remaining cases, i.e., if neither of the conditions $|p| \gg p_c$, $k \ll L$, or $L - k \ll L$ is fulfilled, the $|r_k|$ will not be much smaller than required by (65). A more quantitative illustration of those general features is obtained by introducing Eq. (64) into Eqs. (61) and (62), yielding after a straightforward calculation

$$\sin(r_k) = p^{-1} \sin(p_c r_k + \pi k/L). \quad (69)$$

Together with the constraints in and above Eq. (65), one thus can deduce for large $|p|$ and any $k \in \{1, \dots, L - 1\}$, the asymptotics

$$r_k = p^{-1} \sin\left(\frac{\pi k}{L}\right) \left(1 + \frac{p_c}{p} \cos\left(\frac{\pi k}{L}\right) + \mathcal{O}(p^{-2})\right). \quad (70)$$

Likewise, Eq. (69) implies for $|p| > p_c$ and sufficiently small k/L (which is only possible if $L \gg 1$) that

$$r_k = \frac{1}{p - p_c} \frac{\pi k}{L} (1 + \mathcal{O}(k^2/L^2)), \quad (71)$$

and analogously for sufficiently small $\bar{k}/L$ with $\bar{k} := L - k$ that

$$r_k = \frac{1}{p + p_c} \frac{\pi \bar{k}}{L} (1 + \mathcal{O}(\bar{k}^2/L^2)). \quad (72)$$

Finally, for sufficiently large L , we can approximate p_c in Eq. (63) by unity. After a few steps, one thus obtains from Eq. (69) the large- L asymptotics

$$\tan(r_k) = \frac{p^{-1} \sin\left(\frac{\pi k}{L}\right)}{1 - p^{-1} \cos\left(\frac{\pi k}{L}\right)}. \quad (73)$$

For any given $k \in \{1, \dots, L - 1\}$, there exists a unique solution r_k of this equation together with the constraints in and above Eq. (65). Since $|p^{-1}| < p_c^{-1} < 1$ [see Eq. (63)], one can moreover conclude that this solution must actually satisfy the even stronger bound $|r_k| < \pi/2$ (compared to Eq. (65)), and therefore can be explicitly obtained by acting with the main branch of the function arctan on both sides of Eq. (73). Finally, the denominator in Eq. (73) can always be rewritten as a convergent geometric series. Together with $\arctan(x) = x - x^3/3 + x^5/5 - \dots$ this yields a convenient expansion of

r_k in powers of $p^{-1} \sin(\pi k/L)$ and $p^{-1} \cos(\pi k/L)$, thus systematically generalizing Eq. (70) in the special case $L \gg 1$ and thus $p_c \simeq 1$.

Turning to the case $|p| < p_c$, a similar qualitative discussion as above Eq. (63) applies. The main differences can be briefly summarized as follows. The salient point is that, as p crosses the critical value p_c from above, an additional solution of Eq. (61) appears in the interval between $x = 0$ and the first pole of $f(x)$ at $x = \pi/L$, see also Fig. 1. Likewise, one solution disappears when p crosses the value $-p_c$ from above. Altogether, we thus always obtain L solutions of Eq. (61) if $|p| < p_c$. In the special case $p = 0$, all those solutions must coincide with the zeros of $f(x)$, see item (ii) above. As p moves away from zero, the distance of each solution to the corresponding zero of $f(x)$ must decrease strictly monotonically with p , must be opposite in sign to the sign of p , and cannot exceed the distance between neighboring zeros (see Fig. 1). In other words, we now obtain L pairwise distinct solutions of Eq. (61) of the form

$$\varphi_k = \frac{\pi k + r_k}{L + 1} \quad \text{with } k \in \{1, \dots, L\}, \quad (74)$$

where the r_k are again bounded as in Eq. (65) and are strictly monotonically decreasing functions of p , while their sign must now be opposite to the sign of p . Likewise, the counterparts of Eqs. (66)–(68) now assume the form

$$E_k = \cos\left(\frac{\pi k + r_k}{L + 1}\right), \quad (75)$$

$$U_{kl} = \kappa_k^{-1} \sin\left(\frac{l\pi k + lr_k}{L + 1}\right), \quad (76)$$

$$\kappa_k := \left(\sum_{l=1}^L \sin^2\left(\frac{l\pi k + lr_k}{L + 1}\right)\right)^{1/2} \quad (77)$$

but now for all $k, l \in \{1, \dots, L\}$. As before, the r_k are furthermore seen to become even much smaller than required by (65) in the special cases $|p| \ll 1$, $k \ll L$, or $L + 1 - k \ll L$ (which is only possible for $L \gg 1$), but not in any other case. Finally, upon introducing Eq. (74) into (61), one now finds after a straightforward calculation that

$$\sin(r_k) = p \sin(p_c^{-1} r_k - \pi k/(L + 1)), \quad (78)$$

complemented by the constraints below Eq. (74). We thus recover the same equation as in (69) upon replacing p by $-p^{-1}$, p_c by $-p_c^{-1}$, and L by $L + 1$. The same correspondence is inherited by the results (70)–(72). For small p and any $k \in \{1, \dots, L\}$, one thus obtains

$$r_k = -p \sin\left(\frac{\pi k}{L + 1}\right) \left(1 + \frac{p}{p_c} \cos\left(\frac{\pi k}{L + 1}\right) + \mathcal{O}(p^2)\right). \quad (79)$$

Likewise, one finds for $|p| < p_c$ and sufficiently small k/L that

$$r_k = -\frac{p}{1 + p/p_c} \frac{\pi k}{L + 1} (1 + \mathcal{O}(k^2/L^2)), \quad (80)$$

and analogously for sufficiently small $\bar{k}/L$ with $\bar{k} := L + 1 - k$ that

$$r_k = -\frac{p}{1 + p/p_c} \frac{\pi \bar{k}}{L + 1} (1 + \mathcal{O}(\bar{k}^2/L^2)). \quad (81)$$

Finally, for sufficiently large L we can approximate p_c in Eq. (63) by unity. Similarly as in Eq. (73), one thus can deduce from Eq. (78) the large- L asymptotics

$$\tan(r_k) = -\frac{p \sin\left(\frac{\pi k}{L+1}\right)}{1 - p \cos\left(\frac{\pi k}{L+1}\right)}. \quad (82)$$

As long as $|p| < 1$, the discussion of this result is analogous as below Eq. (73) and therefore not repeated here. The case $|p| = 1$ will be separately considered below. The remaining case $|p| > 1$ is of limited interest. Indeed, any given p with $|p| > 1$ will violate for sufficiently large L our present overall assumption $|p| < p_c = (L + 1)/L$. We thus restrict ourselves to two brief remarks concerning this case $1 < |p| < p_c$. (i) The approximation (82) now becomes questionable since we assumed in its derivation that p_c can be approximated by unity. (ii) This is the only case where the inequality $|r_k| < \pi/2$ (see below Eqs. (73) and (82)) may possibly be violated. A simple example arises for $p \uparrow p_c$ and $k = 1$, where one can readily infer from Fig. 1 that $\varphi_1 \rightarrow 0$ and hence from Eq. (74) that $r_1 \rightarrow -\pi$.

Yet another special case which can be solved exactly is when $|p| = 1$ (note that this still implies $|p| < p_c$). Namely, one can show (see Appendix C) that

$$\begin{aligned} r_k &= -\pi \frac{L + 1 - k}{2L + 1} \quad \text{for } p = 1, \\ r_k &= \pi \frac{k}{2L + 1} \quad \text{for } p = -1 \end{aligned} \quad (83)$$

and $k \in \{1, \dots, L\}$, implying with Eq. (74) that

$$\begin{aligned} \varphi_k &= \pi \frac{k - 1/2}{L + 1/2} \quad \text{for } p = 1, \\ \varphi_k &= \pi \frac{k}{L + 1/2} \quad \text{for } p = -1. \end{aligned} \quad (84)$$

By combining the monotonicity property below Eq. (74) with Eqs. (83), one readily obtains a further refinement of the previously obtained bound $|r_k| < \pi/2$ [see below Eqs. (73) and (82)]. Incidentally, these results for $|p| = 1$ are equivalent to those obtained by Tasaki in Sec. 3.1 of Ref. [38].

Altogether, in the case $|p| < p_c$ we thus found all the L solutions required below Eqs. (40) and (45). On the other hand, in the case $|p| > p_c$ we only found $L - 1$ solutions, i.e., one solution is still “missing.” The latter will be obtained in the next section.

2. Case B: localized modes

According to Eqs. (58) and (59), we have to solve

$$g(y) = \pm p \quad \text{with } y \in \mathbb{R}^+, \quad (85)$$

$$g(x) := \frac{\sinh(x(L + 1))}{\sinh(xL)}, \quad (86)$$

where the plus sign arises when choosing $n = 0$ in Eq. (59) and the minus sign when choosing $n = 1$.

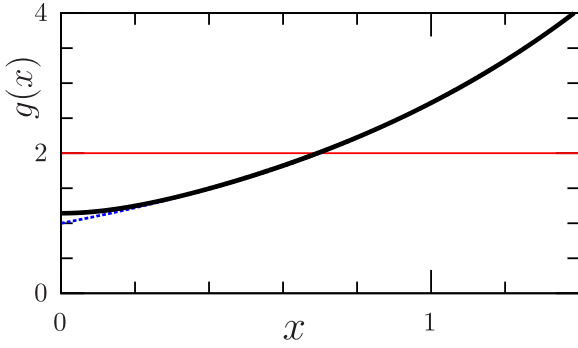


FIG. 2. Black: The function $g(x)$ from Eq. (86) for $x > 0$ (see Eq. (85)) and $L = 7$. Similarly to Fig. 1, the intersection of the black curve with the red horizontal line is the graphical solution of Eq. (85) when choosing $p = 2$. Blue dashed curve: the approximation $g(x) \simeq e^x$ mentioned in the main text.

Restricting ourselves to $x \in \mathbb{R}^+$ [see Eq. (85)], the function $g(x)$ exhibits the following properties (see also Fig. 2). (i) It is strictly monotonically increasing. (ii) $g(x) \rightarrow p_c$ for $x \rightarrow 0$, where p_c is defined in Eq. (63). (iii) $g(x) \sim e^x$ for $x \gg 1/L$ (see also the blue dashed curve in Fig. 2).

From (i)–(iii), one can infer that there exists no solution of Eq. (85) if $|p| \leq p_c$, and exactly one solution if $|p| > p_c$, in accordance with the discussion at the end of the previous section. Moreover, the choice $n = 0$ applies in the case $p > p_c$ and $n = 1$ in the case $p < -p_c$. Denoting this solution for $|p| > p_c$ as y_L , and focusing on large L , we moreover can infer from Eqs. (85), (86), and (iii) the approximation

$$y_L \simeq \ln(|p|) \text{ if } \ln(|p|) \gg 1/L. \quad (87)$$

Note that for large L , the latter condition $\ln(|p|) \gg 1/L$ is equivalent to $|p| - p_c \gg 1/L$. Finally, (59) implies $\varphi_L = y_L$ if $p > p_c$ and $\varphi_L = y_L + i\pi$ if $p < -p_c$. Together with Eqs. (38), (39), (56), (57), and (87), the so far still “missing” solution with index $k = L$ (see end of the previous section) can thus be approximately rewritten for large L and $|p| - p_c \gg 1/L$ as

$$E_L = (p + 1/p)/2, \quad (88)$$

$$U_{Ll} = \sqrt{1 - 1/p^2} (1/p)^{\bar{l}}, \quad (89)$$

where

$$\bar{l} := L - l \quad (90)$$

is the distance of the site l from the right chain-end (at the site L). A more detailed analysis reveals that the relative error of the approximation (88) is on the order of p^{-2L} . Regarding the approximation (89), it is the absolute rather than the relative error which is of foremost interest, and which is found to be on the order of $p^{-(L+1)}$.

Observing that $|1/p| < 1/p_c < 1$ it follows that U_{Ll} is maximal (in modulus) for $l = L$ (chain end) and decreases exponentially with increasing distance $\bar{l}$ from the end. Moreover, for $p > p_c$, the energy in Eq. (87) satisfies $E_L > 1$ and all U_{Ll} in Eq. (88) are positive, whereas for $p < -p_c$, the energy in Eq. (87) satisfies $E_L < -1$ and the U_{Ll} in Eq. (88) exhibit alternating signs [37].

Roughly speaking, that particular solution of type A, which approaches zero and then disappears when p crosses the critical value p_c from below [see discussion above Eq. (74)], may thus be imagined as actually “turning from real to imaginary” and then reappearing as a solution of type B, and likewise when p crosses the value $-p_c$. A more detailed discussion is provided in the next section.

3. The case $|p| \simeq p_c$

If $|p|$ approaches p_c from above, one readily confirms that there are still $L - 1$ solutions of the form (66)–(68), satisfying Eqs. (65) and (69). Concerning the remaining (or “missing”) solution, let us first focus on the case $p = p_c + \epsilon$ with $0 < \epsilon \ll 1$. According to the properties (i) and (ii) below Eq. (86), the solution y of Eq. (85) must approach zero from above as $\epsilon \rightarrow 0$. Moreover, the plus sign must be chosen in (85) and thus $n = 0$ in Eq. (59), implying $\varphi = y$. For sufficiently small ϵ , it furthermore follows that $\varphi \ll L$ and with (56) that $a_l \simeq \varphi^l$, i.e., a_l must be proportional to l . Together with Eqs. (38), (39), and (57), this leads us to the conjecture that the “missing” solution with $k = L$ assumes the form

$$E_L = 1 \quad \text{and} \quad U_{Ll} = \kappa_L^{-1} l \quad \text{if } p = p_c, \quad (91)$$

where $\kappa_L := [\sum_{l=1}^L l^2]^{1/2} = [L(L+1)(2L+1)/6]^{1/2}$. This conjecture can be readily verified by noting that Eq. (91) indeed satisfies Eqs. (43)–(45) [together with Eqs. (38) and (39)] even exactly. Analogously, one finds the exact results [37]

$$E_L = -1 \quad \text{and} \quad U_{Ll} = \kappa_L^{-1} (-1)^l l \quad \text{if } p = -p_c. \quad (92)$$

Without going into the details, we remark that the very same findings could also be deduced in the limit $|p| \uparrow p_c$ from the results in Sec. IV B 1 (case A). Moreover, for any given L with $L \gg 1$ one can show that Eqs. (91) and (92) still remain very good approximations as long as $||p| - p_c| \ll 1/L$. [We may also recall that the case $|p| = 1$ corresponds to $||p| - p_c| = 1/L$ and is solved exactly by Eqs. (75)–(77) with r_k from Eq. (83).]

C. Interim summary and discussion

As detailed below Eq. (40), our basic Eqs. (29) or (40) may be viewed as an L -dimensional Hermitian matrix eigenvalue problem. For $|p| < p_c$, the solutions (L eigenvalues and eigenvectors) are given by Eqs. (74)–(77), where the r_k are determined via Eqs. (78) and (65). Likewise, for $|p| \geq p_c$, there are $L - 1$ solutions of the form (66)–(68), where the r_k are determined via Eqs. (69) and (65). In addition, there is one more solution which is of the form (88) and (89) if $|p| > p_c$ and of the form (91) and (92) if $|p| = p_c$.

In view of Eq. (65), the quantities r_k in Eqs. (66) and (75) become negligible for sufficiently large L . However, it is important to realize that those r_k are generally *not negligible* in Eqs. (67) and (76) as soon as the indices l are comparable in order of magnitude to L [since the quantities $l r_k / L$ on the right-hand side of Eqs. (67) and (76) are no longer small]. Exceptions are asymptotically large or small values of $|p|$ since all r_k then approach zero according to Eqs. (70) and (79), respectively. Further very important exceptions are the normalization constants κ_k from (68) and (77). Namely, as

shown in Appendix D, they can be approximated for large L as

$$\kappa_k = \sqrt{L/2}, \quad (93)$$

where the omitted relative error approaches zero for $L \rightarrow \infty$.

Put differently, the presence of an impurity ($p \neq 0$) at the right chain-end (at $l = L$) entails a marked asymmetry of the matrix elements U_{kl} with respect to the second index l (while k is arbitrary but fixed). For instance, focusing on $|p| < p_c$ and setting formally $l = 0$ or $l = L + 1$, the matrix elements in Eq. (76) are zero in the former and nonzero in the latter case [namely, $U_{kL+1} \sim \sin(r_k)$]. An analogous asymmetry—governed by r_k —arises when comparing $l = 1$ with $l = L$ or when $|p| > p_c$ [see Eq. (67)].

Returning to the above mentioned L -dimensional Hermitian matrix eigenvalue problem, its solutions may also be viewed as L eigenvalues of the form (38) and L eigenvectors $\vec{a}$ with components a_l of the form (39) [see also below Eq. (40)]. From Eqs. (76), (77), and (93), one can infer that, for any given $k \in \{1, \dots, L\}$, most of those components assume values which are of comparable order of magnitude in the case $|p| < p_c$. Henceforth, we will thus often employ the common notion of *delocalized* (or *extended*) modes (or eigenvectors) for this type of solutions (see Ref. [39] and further references therein). In the same vein, there are $L - 1$ delocalized solutions in the case $|p| > p_c$ according to Eqs. (67), (68), and (93), and likewise for $|p| = p_c$ (see Sec. IV B 3).

On the other hand, the components of the L th eigenvector in Eq. (89) are largest (in modulus) at the right chain-end, corresponding to $\bar{l} = 0$ in Eq. (90), and decrease exponentially with increasing distance $\bar{l}$ from the chain-end. Accordingly, we will often refer to such solutions as *localized* modes [39]. More precisely speaking, Eq. (89) amounts to a strongly (exponentially) localized solution, while the corresponding solution for $|p| = p_c$ in (92) is weakly localized in the sense that the components only decrease algebraically with increasing distance from the right chain-end.

D. Absence of thermalization and strong violation of the ETH for $|p| > p_c$

In this section, we derive the first analytical key results of our present paper, namely nonthermalization after a local quench with the property $|p| > p_c$, and a concomitant strong ETH violation (see also Sec. I).

As explained below Eq. (19), in order to show the absence of thermalization, it is sufficient that the long-time average of $\bar{C}_{VA}(t)$ does not approach zero for large L . The latter property is derived in the next section, followed by a discussion of its implications in Sec. IV D 2.

1. Derivation

Focusing on $|p| > p_c$ and $L \gg 1$, we observed above Eq. (64) that the quantities φ_k in Eq. (64) are pairwise distinct and contained in the interval $(0, \pi)$, implying that the E_k in Eq. (66) are pairwise distinct and contained in the interval $(-1, 1)$, where $k \in \{1, \dots, L - 1\}$. Moreover, from Eq. (88) and the discussion above Eq. (88) it follows that E_L is larger than unity in modulus. Altogether, it follows that the E_k are pairwise distinct for all $k \in \{1, \dots, L\}$. As a consequence,

the long-time average of the quantities in Eq. (37) is given according to Eq. (18) by $e_{jk}(t) = \delta_{jk}$. From Eq. (35), we thus can conclude that

$$\overline{\bar{C}_{VA}(t)} = \sum_{k=1}^L |U_{kL}|^2 |U_{k\alpha}|^2 f_{kk}, \quad (94)$$

where we set $v = L$ according to Eq. (42). With the help of the auxiliary quantities

$$R_{L,\alpha} := \sum_{k=1}^{L-1} |U_{kL}|^2 |U_{k\alpha}|^2 f_{kk}, \quad (95)$$

$$S_{L,\alpha} := |U_{LL}|^2 |U_{L\alpha}|^2 f_{LL}, \quad (96)$$

we can rewrite Eq. (94) as

$$\overline{\bar{C}_{VA}(t)} = R_{L,\alpha} + S_{L,\alpha}. \quad (97)$$

Moreover, by employing l'Hopital's rule to evaluate the right-hand side of Eq. (36) in the limit $E_j \rightarrow E_k$, we can conclude that

$$f_{kk} = \frac{1}{4 \cosh^2(\beta E_k/2)}. \quad (98)$$

Our next goal is to derive upper and lower bounds for the quantity in Eq. (95). In a first step, we can infer from Eq. (98) that $0 < f_{kk} \leq 1/4$. Furthermore, by observing Eq. (67) and the large- L approximation (93) it follows that $|U_{kl}|^2 \leq 2/L$ for all $k \in \{1, \dots, L - 1\}$ and $l \in \{1, \dots, L\}$. Altogether, we thus can conclude from (95) that

$$R_{L,\alpha} \in [0, 1/L]. \quad (99)$$

Turning to the quantity in Eq. (96), we can exploit Eqs. (88), (89), and (98) to infer

$$S_{L,\alpha} := \left(1 - \frac{1}{p^2}\right)^2 \left(\frac{1}{p^2}\right)^{\bar{\alpha}} \frac{1}{4 \cosh^2\left(\beta \frac{p+p^{-1}}{4}\right)}, \quad (100)$$

where $\bar{\alpha} := L - \alpha$. [Incidentally, the invariance of Eq. (100) under a sign change of p is in accordance with the general symmetry considerations around Eq. (41).]

Observing Eq. (99), we thus can conclude that the long-time average in Eq. (97) converges to $S_{L,\alpha}$ from Eq. (100) for large L (and fixed $\bar{\alpha}$), which in turn is generically nonzero.

2. Discussion

The latter finding of a nonvanishing long-time average in Eq. (97) implies the absence of thermalization for the observable $A = s_\alpha^z$ [see below Eq. (19)]. With Eqs. (19) and (20), we furthermore obtain the approximation

$$\overline{\langle s_\alpha^z \rangle_t} - \langle s_\alpha^z \rangle_{\text{th}} = g\beta S_{L,\alpha}, \quad (101)$$

where $S_{L,\alpha}$ is given by Eq. (100), and where $|p| > p_c$ is tacitly taken for granted. As expected, the nonthermalization effect is most pronounced if the observable-site α coincides with the site $v = L$ of the perturbation [see Eqs. (8) and (42)], and decreases exponentially with increasing $\bar{\alpha} := L - \alpha$.

We also remark that an arbitrarily small (nonzero) perturbation strength g in (101) is sufficient for nonthermalization provided the prequench impurity strength γ is notably larger (in modulus) than $1/2$, see also the discussion below Eq. (8)

and the definitions (17) and (63). Moreover, for small g , all our analytical approximations become asymptotically exact, as discussed below Eq. (16).

Finally, these conclusions regarding nonvanishing long-time averages in combination with the considerations in Secs. IID immediately imply that our present model with $|p| > p_c$ must exhibit a strong violation of the ETH in the sense that neither the strong nor the weak ETH is satisfied. An alternative, more direct derivation of the same result is provided in Appendix E.

Obviously, the above finding of nonthermalization and strong ETH violation for $|p| > p_c$ has its origin in the contribution of the localized mode (see Sec. IV C) with index $k = L$ to the sum in Eq. (94). Accordingly, the absence of such a mode in the case $|p| < p_c$ rules out a similar conclusion. The same applies to the weakly localized case $|p| = p_c$, as can be inferred from the results in Sec. IV B 3 or by taking the limit $|p| \rightarrow p_c = (L + 1)/L$ in Eq. (100).

We finally mention that the thermal expectation values $\langle s_L^z \rangle_{\text{th}}$ do *not* exhibit any kind of “transition” at $|p| = p_c$ (see Appendix G for the details).

E. Numerical methods and results

The first purpose of this section is to illustrate and complement the analytical predictions and approximations from the previous sections by quantitative numerical examples. On the one hand, we therefore solved Eqs. (1)–(11) by means of standard, numerically exact diagonalization methods. As usual, such computations are only practically feasible for relatively small system sizes L . [On the machines available to us, up to $L = 24$ was doable with reasonable effort and by taking advantage of dynamical typicality concepts.] Furthermore, we numerically evaluated the analytical approximation (15) by exploiting the exact analytical result from Eqs. (35)–(37), where the energies E_k and the unitary matrix elements U_{kl} were obtained by numerically solving Eq. (29) [or the equivalent Eqs. (43)–(45)]. Finally, we also found a way of how those energies E_k and matrix elements U_{kl} can be exploited to numerically evaluate Eqs. (1)–(11) up to quite large L values [for instance, $L = 10^4$ turned out to be still easily doable]. A more detailed account of this numerical method is provided in Appendix F.

The second purpose of this section is to “gauge” how well the behavior in the thermodynamic limit $L \rightarrow \infty$ can be extrapolated from the numerical data up to $L = 24$, i.e., by means of the above-mentioned standard numerical methods. The underlying rationale is as follows: In our present explorations of the XX model, we are able to compare the latter numerical data with our approximate or even exact analytical findings, as well as with the above mentioned more sophisticated numerical methods for much larger L -values. However, in our later explorations of the XXZ model, the only remaining tool will be the standard numerical methods. Thus only data up to $L = 24$ will be available for the extrapolation to the thermodynamic limit. In doing so, it seems reasonable to expect and will be tacitly taken for granted that the quality of such an extrapolation is comparable to that in our present case of the XX model.

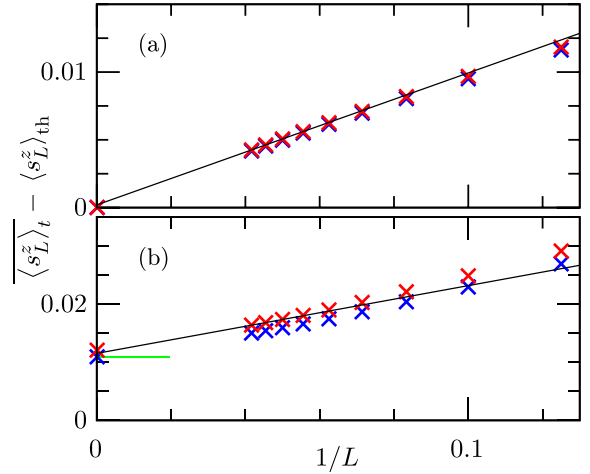


FIG. 3. Red crosses: Numerically exact time-averaged expectation values $\langle s_L^z \rangle_t - \langle s_L^z \rangle_{\text{th}}$ versus $1/L$ for the XX model from Eqs. (1)–(11) with parameter values $J_{\perp} = 1$, $J_z = 0$, $v = \alpha = L$, $\beta = 1$, $\gamma = 0$, and $g = 0.3$ in (a), $g = 0.6$ in (b). Hence, $p = 0.6 < p_c$ in (a) and $p = 1.2 > p_c$ in (b), see Eqs. (17) and (63). Blue crosses: Corresponding analytical approximations from Eq. (15), see also main text. The leftmost crosses correspond to $L = 10^4$, followed by $L = 24, 22, \dots, 10, 8$. The black lines are a guide to the eye, representing a linear extrapolation towards $1/L = 0$ based on the red crosses with $L \leq 24$. The closeness of the lines to the red crosses at $L = 10^4$ thus quantifies the reliability of such an extrapolation. The green bar in (b) indicates the analytical approximation for $L \rightarrow \infty$ from Eqs. (100) and (101).

The red crosses in Fig. 3 exemplify the time-averaged expectation values $\langle A \rangle_t - \langle A \rangle_{\text{th}}$ for $A = s_L^z$, obtained by the above-mentioned numerical solutions of the XX model with parameter values as specified in the figure caption. In other words, the prequench Hamiltonian H_0 appearing in the initial Gibbs state (3) is given by the basic XX-Hamiltonian from Eq. (24) with $p = 0$ (no impurity, see also Eq. (17)). Similarly, the postquench Hamiltonian is given by Eq. (24) with $p = 0.6$ in (a) and $p = 1.2$ in (b), i.e., it exhibits an impurity at the right chain-end ($V = s_L^z$) as specified in and around Eq. (42). According to Eq. (63) this means that $p < p_c$ in (a) and $p > p_c$ in (b).

Comparing the blue and red crosses in Fig. 3 illustrates that the approximation (15) is very accurate in (a) and notably less accurate in (b), in accordance with the general analytical predictions below Eq. (16). More precisely speaking, the value of $g\beta = 0.3$ in (a) is still not really small, and all the more so for the value $g\beta = 0.6$ in (b). We have purposefully made this choice in order to obtain some still clearly visible differences between the blue and red crosses. In other words, Fig. 3 illustrates that the analytical error bound below Eq. (16) is, in general, not very tight. We also validated (not shown) that the differences indeed become even much smaller upon decreasing $g\beta$, as predicted below Eq. (16). Another noteworthy observation is that the approximation (15) obviously is (again as analytically predicted) not restricted to large system sizes L .

The straight black lines in Fig. 3 depict the extrapolation of the numerically exact results (red crosses) for $L \leq 24$ into

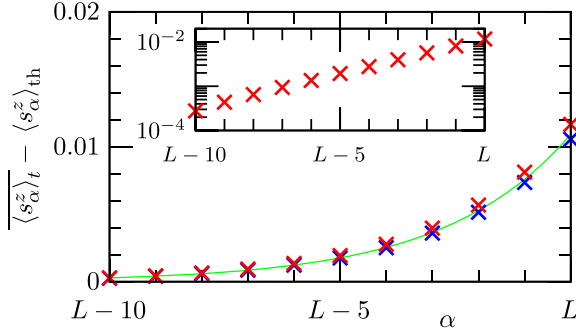


FIG. 4. Time-averaged expectation values $\overline{\langle s_\alpha^z \rangle_t} - \langle s_\alpha^z \rangle_{\text{th}}$ vs $\alpha \in \{L-10, \dots, L\}$ for the same XX model as in Fig. 3(b). Red crosses: Extrapolations of the numerically exact results for $L = 8, 10, \dots, 24$ to $L \rightarrow \infty$ by means of the same procedure as indicated by the black lines in Fig. 3. In particular, the red cross for $\alpha = L$ corresponds to the black line in Fig. 3(b) at $1/L = 0$. Blue crosses: analogous extrapolations based on the approximation from Eq. (15). Green curve: corresponding approximations from Eqs. (100) and (101). (Inset) Semilogarithmic plot of the same numerical results as in the main plot.

the regime $L > 24$. The main point is that these extrapolations are still quite close to the “true” numerical values at $L = 10^4$ (leftmost red crosses). We thus can conclude that already the numerically exact results up to $L = 24$ admit a quite faithful extrapolation of the behavior in the thermodynamic limit (see also second paragraph of this section). In other words, the extrapolation would change very little if also the leftmost cross at $L = 10^4$ would be taken into account. Moreover, such an even better extrapolation would hit the origin even more closely in Fig. 3(a) but definitely not in (b). All this quite convincingly confirms the absence of thermalization for $|p| > p_c$ but not for $|p| < p_c$ [40], as analytically predicted in the previous section. Finally, the practically perfect agreement of the green bar and the leftmost blue cross in Fig. 3(b) illustrates the very high accuracy of the analytical approximation from Eqs. (100) and (101).

Figure 4 was obtained by similar extrapolations to asymptotically large L as in Fig. 3, but now depicting results for more general observables $A = s_\alpha^z$ with α close to L (right chain-end). Moreover, we confined ourselves to the case $g = 0.6$, corresponding to panel (b) in Fig. 3 with $p = 1.2 > p_c$. (Similarly to panel (a), $g = 0.3$ yields identically vanishing results for $L \rightarrow \infty$). Once again, the analytical approximations from Eq. (15) (blue) and from Eqs. (100) and (101) (green) are seen to work quite well. In particular, they faithfully reproduce the numerically observed “localization” of nonthermalization near $\alpha = L$, as predicted below Eq. (101) and discussed in more detail in Sec. IV G. The inset as well as the green curve in the main plot corroborate an exponential decay of the numerical results with $L - \alpha$, as analytically predicted by Eq. (100).

F. Temporal relaxation behavior

While the focus in the previous sections was on time-averaged expectation values, the present section provides

some analytical approximations as well as numerical results regarding their time dependence.

1. Analytical approximations

Similarly as in Sec. IV D [see also discussion below Eq. (16)], we take the approximation (15) for granted and focus on the behavior of the quantity $\tilde{C}_{VA}(t)$ from Eq. (16). Moreover, the perturbations V and observables A are again assumed to be of the specific form (8), (11), and (42), hence we can employ the exact result (35) as our starting point.

For simplicity, we focus on the most interesting case

$$\alpha = L, \quad (102)$$

meaning that both the perturbation V and the observable A are given by the spin s_L^z at the right chain-end. Moreover, we focus on sufficiently high temperatures such that

$$|\beta E_k| \ll 1 \quad \text{for all } k \in \{1, \dots, L\}. \quad (103)$$

Therefore all f_{jk} in Eq. (36) can be approximated by $1/4$, and the double sum in Eq. (35) can be rewritten as the product of two simple sums. In those cases where explicit analytical approximations for E_k and U_{kl} are available (see Sec. IV B), and under the additional assumption that

$$L \gg 1, \quad (104)$$

those sums can be furthermore approximated very well in terms of Bessel functions by means of a very similar line of reasoning as, for instance, in Ref. [13]. Thus, omitting the detailed calculations, the final results are as follows.

For $|p| \ll p_c$ [where $p_c \simeq 1$ according to Eqs. (63) and (104)], we can exploit Eq. (79) to deduce the approximation

$$\tilde{C}_{VA}(t) \simeq \frac{b(t) + p^2 c(t)}{4} \quad \text{for } |p| \ll 1, \quad (105)$$

$$b(t) := [J_0(t) + J_2(t)]^2, \quad (106)$$

$$c(t) := [J_1(t) + J_3(t)]^2 - 2[J_0(t) + J_2(t)][J_2(t) + J_4(t)], \quad (107)$$

where $J_n(t)$ are the Bessel functions of the first kind. Similarly, by exploiting Eq. (83), one obtains

$$\tilde{C}_{VA}(t) \simeq \frac{J_0^2(t) + J_1^2(t)}{4} \quad \text{for } |p| = 1. \quad (108)$$

Finally, one can utilize Eq. (69) to infer

$$\tilde{C}_{VA}(t) \simeq \frac{1 - 2p^{-2}d(t)}{4} \quad \text{for } |p| \gg 1, \quad (109)$$

$$d(t) := 1 - [J_0(t) + J_2(t)] \cos(E_L t), \quad (110)$$

where E_L is approximately given by Eq. (88). Note that for large values of $|p|$, as required in Eq. (109), also the energy E_L in Eq. (88) becomes large (in modulus), hence the condition (103) becomes quite restrictive with respect to β .

The most important observation is that all Bessel functions $J_n(t)$ approach zero for large t . Hence, Eqs. (105) and (108) approach zero for large t , while the long time-limit in Eq. (109) agrees with the long-time average from Eq. (100) [wherein $\bar{\alpha} = 0$ and the last factor approaches $1/4$ according to Eqs. (88) and (103)].

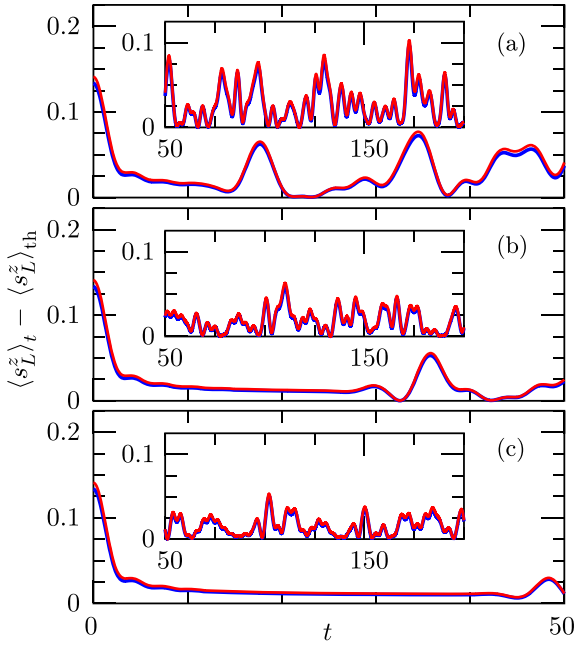


FIG. 5. Red: numerically exact time-dependent expectation values $\langle s_L^z \rangle_t - \langle s_L^z \rangle_{\text{th}}$ for the same XX model as in Fig. 3(b) with $L = 8, 16$, and 24 in (a), (b), and (c), respectively. Blue: corresponding analytical approximations from Eq. (15). Main plots: initial relaxation behavior for $t \in [0, 50]$. (Insets) Long-time behavior for $t \in [50, 200]$. The blue curves are sometimes nearly covered by the red ones.

Second, we recall that $\tilde{C}_{VA}(t)$ must be an even function of β and of p , see below Eqs. (37) and (41), respectively. Our present approximations are in accordance with these predictions. In particular, they are independent of β , i.e., corrections of order β^2 have been neglected [see also Eq. (103)]. Moreover, the approximation (105) includes terms up to second order in p , i.e., corrections of order p^4 have been neglected. Likewise, corrections of order $1/p^4$ have been neglected in Eq. (109). A quantification of the finite- L corrections [cf. Eq. (104)] is analytically less obvious (but numerically easy, see next section).

A more detailed discussion by exploiting the well-known properties of the Bessel functions is straightforward but not of central interest with respect to the main issues of our present work. Likewise, a generalization to other values of α than in Eq. (102) is readily feasible in principle, but the analytical expressions would become even more involved than in the above findings. Finally, going beyond the approximations (103) and (104) and beyond the p values in Eqs. (105), (108), and (109) becomes very arduous by analytical means.

2. Numerical examples

Here we illustrate the detailed temporal relaxation behavior by employing the same numerical methods as in Sec. IV E. Moreover, we compare the analytical approximations from the previous section with such numerically exact results.

The red curves in Fig. 5 exemplify the numerical expectation values $\langle A \rangle_t - \langle A \rangle_{\text{th}}$ for $A = s_L^z$ and the same XX model as in Fig. 3(b). Their very good agreement with the blue curves

in Fig. 5 confirms once again (see also Sec. IV E) that the approximation (15) is very accurate, and works practically equally well for largely arbitrary system sizes L and times t . Likewise, we confirmed (not shown) that the agreement becomes even better for smaller values of $g\beta$, as predicted below Eq. (16).

Another interesting observation in Fig. 5 is that the curves seem to be (practically) independent of L as long as the time t is smaller than about $1.75L$ (in our present units), while exhibiting quite notable and strongly L -dependent pseudorandom “fluctuations” for even larger times t . In other words, moderately large L values (such as in Fig. 5) already emulate very well the behavior in the thermodynamic limit $L \rightarrow \infty$ up to times of about $1.75L$. Indeed, our numerically exact results for $L = 10^4$ would be indistinguishable for $t < 1.75L$ from the blue curves in Fig. 5 and are therefore not shown. The intuitive physical explanation is that the system’s behavior after a local quench at the right chain-end needs some time (proportional to L) to “notice” that the chain is of finite rather than infinite length. A more detailed explanation and additional examples of these well-known general features can be found, for instance, in Ref. [13].

The insets of Fig. 5 indicate that the typical amplitudes of the above mentioned pseudorandom fluctuations for $t > 1.75L$ decrease with increasing L . (Incidentally, also the mean-value of those fluctuations depends on L , see also Fig. 3.) A much more detailed analytical and numerical investigation of this issue has been carried out in Ref. [13] for a somewhat different model. We found that largely the same observations and conclusions are also recovered for our present model, and hence are not repeated here. The main result is that the behavior for a given, large but finite system size L at very large times t cannot be easily related to the behavior at a fixed, large but finite time t for very large systems sizes L . Yet, if both t and L approach infinity, the sequence of the limits becomes irrelevant. Moreover, the behavior in this double-limit can already be recovered in very good approximation for relatively small L when focusing on times $t < 1.75L$.

We emphasize that our analytical demonstration of non-thermalization in Sec. IV D and its numerical confirmation in Sec. IV E remain entirely unaffected by all these quite subtle large- t versus large- L issues.

Finally, we turn to the comparison of our analytical approximations from the previous section with numerical examples, see Fig. 6. Note that $p = 0.2 < p_c$ in (a), $p = 1 \simeq p_c$ in (b), and $p = 2 > p_c$ in (c), where $p_c = (L + 1)/L = 1.0001$, see also Eqs. (17) and (63). The black curves in Fig. 6 exemplify the approximations from Eqs. (105)–(110). In order to fulfill the requirement (103) in those approximations, we have chosen in Fig. 6 a smaller value of β than in Fig. 5. While the agreement between the blue and black curves is very good in (a) and (b), the deviations in (c) are somewhat larger. The main reason seems to be that the condition $|p| \gg 1$ in Eq. (109) is not yet very well fulfilled for the choice of $p = 2$ in Fig. 6(c). We numerically found that the agreement indeed becomes better upon further increasing p (not shown). On the other hand, for larger p -values, correspondingly smaller β -values must be chosen in order to still fulfill Eq. (103). Moreover, upon increasing p the overall temporal variations become smaller

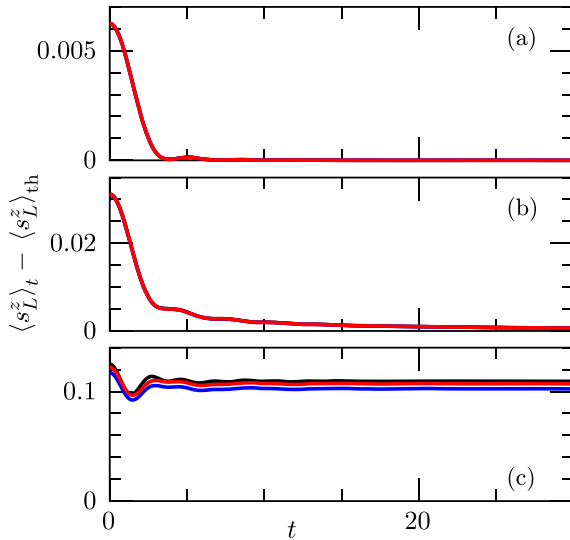


FIG. 6. Red: numerically exact expectation values $\langle s_L^z \rangle_t - \langle s_L^z \rangle_{\text{th}}$ for the XX model from Eqs. (1)–(11) with parameter values $J_\perp = 1$, $J_z = 0$, $\nu = \alpha = L = 10^4$, $\beta = 1/4$, $\gamma = 0$, and $g = 0.1, 0.5$, and 2 in (a), (b), and (c), respectively. Blue: corresponding analytical predictions (15). Black: corresponding approximations from Eqs. (105), (108), and (109) in (a), (b), and (c), respectively. The blue and black curves are (almost) covered by the red ones in (a) and (b).

and smaller, as can be most easily deduced from Eq. (109). In other words, the choice $p = 2$ in Fig. 6(c) amounts to a compromise between a nearly trivial time-dependence and a breakdown of the analytical approximation (109).

Note that we restricted ourselves in Fig. 6 to the regime $t < 1.75L$ (see also the discussion above). As expected, in the regime $t > 1.75L$, one finds (not shown) that the black curves will remain (practically) constant, while the red and blue curves will exhibit the usual pseudorandom fluctuations (see above), whose typical amplitudes are, however, already very small due to the quite large value of $L = 10^4$. As detailed in Ref. [13], this is accompanied by a breakdown of the approximation mentioned below Eq. (104).

Physically speaking, the case $p > p_c$ in Fig. 6(c) amounts to yet another example of nonthermalization (nonzero long-time average). Likewise, the case $p < p_c$ in Fig. 6(a) gives rise to a vanishing long-time average [40]. Finally, the case $p = p_c$ in Fig. 6(b) may be viewed as a “critical point,” exhibiting a particularly slow relaxation towards zero.

G. Signatures of localization

As detailed at the end of Sec. IV C, for $|p| \geq p_c$ a so-called localized mode (with index $k = L$) arises, whose characteristic signature is that U_{Ll} in Eq. (89) or Eq. (91) decreases (in modulus) with increasing distance $\bar{l} := L - l$ from the right chain-end (exponentially for $|p| > p_c$ and algebraically for $|p| = p_c$). Moreover, the appearance of such a localized mode is essential for the absence of thermalization, as observed at the end of Sec. IV D 2. It is however important to realize that this notion of localization refers to the auxiliary eigenvalue problem in and around Eq. (40). The latter, in turn, arises by mapping the original XX model (24) by means of a

Jordan-Wigner transformation to an equivalent model of free fermions, see Eq. (28). Since the same kind of transformation will *not* be possible for our later considered XXZ model, also such a notion of localization will be meaningless as it stands, and thus needs to be adapted in some suitable way.

Therefore we first address the question whether and how these localization features of the Jordan-Wigner transformed model manifest themselves already in the original XX model from Eq. (24). Two particularly important such manifestations are obviously the absence of thermalization and the strong violation of the ETH from Sec. IV D. But are there also some immediate signatures of “localization” already in the original Hamiltonian (24)?

To begin with, let us consider those eigenvectors $|\vec{b}\rangle$ of H [see in and around Eq. (31)] for which the general definition (30) takes the particularly simple form of a “one-particle excitation” $|k\rangle := f_k^\dagger |0\rangle$ with an arbitrary but fixed $k \in \{1, \dots, L\}$. Observing that $f_k^\dagger = \sum_{l=1}^L U_{kl}^* c_l^\dagger$ according to Eq. (27), exploiting Eq. (25) to infer $c_l^\dagger = \sigma_l^+ Z_l$, and noting that $Z_l |0\rangle = |0\rangle$ [see below Eq. (29)], we thus can conclude that

$$|k\rangle = \sum_{l=1}^L U_{kl}^* \sigma_l^+ |0\rangle. \quad (111)$$

Recalling the definition of $|0\rangle$ below Eq. (29) it follows that $\sigma_l^+ |0\rangle$ may be viewed as a “one-spin excitation,” i.e., a product state where the l th spin points “up” and all other spins point “down.” Accordingly, $|k\rangle$ in Eq. (111) thus represents a linear combination of all possible one-spin excitations with coefficients U_{kl}^* . Choosing $k = L$, the above mentioned localization properties of U_{Ll} then translate into a localization property of $|L\rangle$ in the sense that one-spin excitations near the right chain-end contribute with a much larger weight U_{Ll} than all the others.

Analogously, we may consider any eigenstate in Eq. (30) (apart from $|0\rangle$) as some n -particle excitation of the general form

$$|k_1, \dots, k_n\rangle := f_{k_1}^\dagger \cdots f_{k_n}^\dagger |0\rangle \quad (112)$$

with $k_1, \dots, k_n \in \{1, \dots, L\}$ and $k_1 < k_2 < \dots < k_n$. Similarly as above, one thus can conclude (see Appendix A in Ref. [13]) that

$$|k_1, \dots, k_n\rangle = \sum' u(l_1, \dots, l_n) \sigma_{l_1}^+ \cdots \sigma_{l_n}^+ |0\rangle, \quad (113)$$

where $\sum'$ indicates a sum over all $l_1, \dots, l_n \in \{1, \dots, L\}$ with $l_1 < l_2 < \dots < l_n$ and thus consists of $\binom{L}{n}$ summands. Furthermore,

$$u(l_1, \dots, l_n) := \sum_{\Pi} \tau(\Pi(\mathbf{l})) U_{k_1 l_{\Pi(1)}}^* \cdots U_{k_n l_{\Pi(n)}}^*, \quad (114)$$

where the sum is meant to run over all permutations Π of $\{1, \dots, n\}$ and thus consist of $n!$ summands, and where $\tau(\mathbf{l})$ is either $+1$ or -1 , but for the rest depends in a very complicated way on $\mathbf{l} := (l_1, \dots, l_n)$, ultimately caused by the anticommutation relations mentioned below Eq. (25).

Similarly as before, the last factors $\sigma_{l_1}^+ \cdots \sigma_{l_n}^+ |0\rangle$ in Eq. (113) may now be viewed as “ n -spin excitations.” Moreover, one expects that the localization properties of U_{Ll} somehow enter the game if $k_n = L$. However, the large num-

ber of summands in Eq. (113) and the complicated form of the coefficients in Eq. (114) make a more tangible physical interpretation quite difficult. Therefore we now turn to the signatures of localization, which do not manifest themselves directly in the system's energy eigenstates, but rather in certain characteristic features of some suitably chosen expectation values.

A first such signature arises for that specific eigenvector $|\vec{b}\rangle$ whose components are of the particular form $b_k = \delta_{kL}$ (and which thus coincides with the one-particle excitation $|L\rangle$ from above). Namely, its expectation values for the observables $A = s_\alpha^z + 1/2$ [see also Eq. (11)] may be viewed as being localized near the right chain-end (at $\alpha = L$), as can be inferred from Eq. (E1) in Appendix E. However, this only concerns the above very special energy eigenstate $|\vec{b}\rangle$, whose energy is moreover located somewhere “in the middle of the spectrum of H ” according to Eq. (32). (In particular, it is far from the ground state.) For more general eigenstates $|\vec{b}\rangle$, i.e., many-particle excitations with $b_k = 1$ not only for $k = L$, the traces of the localization properties of U_{Li} become less clean due to the additional “pseudorandom” summands $|U_{ki}|^2$ with $k < L$, see also Eqs. (67), (93), and (E1).

A second signature consists in the fact that the strong violation of the ETH is most pronounced for small $\bar{\alpha}$ values, i.e., near the right chain-end, as discussed in Appendix E around Eq. (E4). A third signature arises by observing that the absence of thermalization from Sec. IV D may again be viewed as being localized near the right chain-end according to Eqs. (100) and (101). A quantitative numerical example is provided in Fig. 4.

Note that the first two above signatures are of rather theoretical character in the sense that properties of single energy eigenstates are quite difficult to observe in an experimental many-body system. The third one is experimentally unproblematic but is of a rather “indirect” character in the sense that it admits little insight into the basic physical mechanism behind it.

In any case, the most fundamental signature of localization, namely the existence of a localized mode U_{Li} , seems hardly seizable beyond the very special class of systems which can be mapped to an equivalent model of free fermions. On the other hand, the second and third above signatures are independent of whether or not such a mapping is available. Moreover, they are in fact very closely related to each other via our key relations (20) and (22).

Finally, it also seems noteworthy that the thermal expectation values $\langle s_\alpha^z \rangle_{\text{th}}$ (see also Appendix G) do *not* exhibit any signature of the onset of localization when p exceeds the critical value p_c .

V. THE XXZ MODEL WITH AN END-IMPURITY

The XXZ model may be viewed as a generalization of the XX model from Eq. (24) when abandoning the requirement $J_z = 0$ in Eq. (23), i.e., the Hamiltonian is now of the form

$$H = \sum_{l=1}^{L-1} (s_{l+1}^x s_l^x + s_{l+1}^y s_l^y + J_z s_{l+1}^z s_l^z) + \frac{p}{2} s_v^z, \quad (115)$$

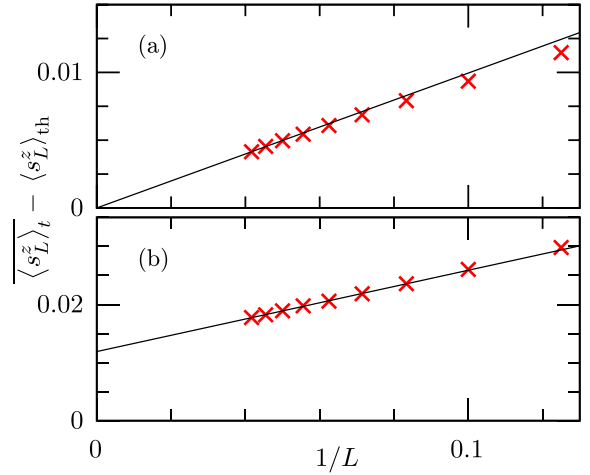


FIG. 7. Same as Fig. 3 but now for the corresponding XXZ model with $J_z = 0.3$ in Eq. (115).

see also Eqs. (1), (2), (5), (8), and (17). Moreover, we focus again on the case of an end-impurity as specified in and around Eq. (42). The main goal of this section is to show that qualitatively similar results as for the XX model are also recovered for the XXZ model.

To the best of our knowledge, a pertinent extension of the general analytical framework from Sec. III is not available for our present XXZ model with an impurity in Eq. (115). Hence, we confine ourselves to purely numerical explorations, analogous to those in Secs. IV E and IV F 2.

In Fig. 7, we show the same type of numerically exact time-averaged expectation values as in Fig. 3, but now for the XXZ model (115) with $J_z = 0.3$ instead of the XX model (corresponding to $J_z = 0$). Moreover, the numerical results for $L = 10^4$ (leftmost crosses in Fig. 3) as well as analytical approximations (blue crosses and green bar in Fig. 3) are no longer available in Fig. 7 (see also previous paragraph and Sec. IV E). Apart from that, the numerical findings in Fig. 7 are indeed quite similar to those in Fig. 3. Finally, we recall the remarks in Sec. IV E (paragraphs 2 and 4 therein) concerning the reliability of our large- L extrapolations by means of the black lines. Altogether, Fig. 7(b) thus provides once again very convincing numerical evidence that the system does not exhibit thermalization after a local quantum quench, see also the more detailed discussion of this issue in Sec. IV E.

As usual (see Sec. II D), once the absence of thermalization has been established for a given system, we can conclude that the system also must exhibit a strong violation of the ETH. Moreover, it seems reasonable to expect that the second and third main signatures of localization from Sec. IV G will be handed down from a nonthermalizing XX to the corresponding XXZ model as well. A numerical confirmation is provided by Fig. 8.

Likewise, Fig. 9 is the counterpart of Fig. 5, but now with $J_z = 0.3$ instead of $J_z = 0$, and without any analytical approximations (blue and black curves in Fig. 5). For the rest, the numerically exact results (red curves) are again qualitatively and even quantitatively quite similar in the two figures for small-to-moderate times with $t \leq 1.75L$, see also Sec. IV F 2. On the other hand, the pseudorandom fluctuations

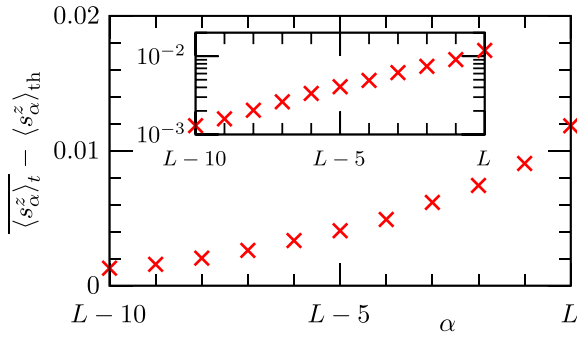


FIG. 8. Same as Fig. 4 but now for the corresponding XXZ model with $J_z = 0.3$ in Eq. (115).

for $t > 1.75L$ in Fig. 9 are still qualitatively similar as in Fig. 5, but quantitatively much weaker [41]. Such quantitative differences have also been reported in related previous investigations. Without going into the details, these differences can be traced back to the fact that we are dealing with so-called interacting and noninteracting integrable models in the case of our present XXZ and XX models, respectively [31].

A more detailed and systematic numerical exploration of how all these various features of the XXZ model depend on J_z , and possibly also on g , γ , L , and β , is a quite interesting issue in its own right, which goes beyond the scope of our present work (see also Sec. VII).

VI. INNER IMPURITIES

A. The XX model with an inner impurity

For the sake of simplicity, we will mainly focus on *odd chain lengths* L and on impurities and perturbations s_v^z in

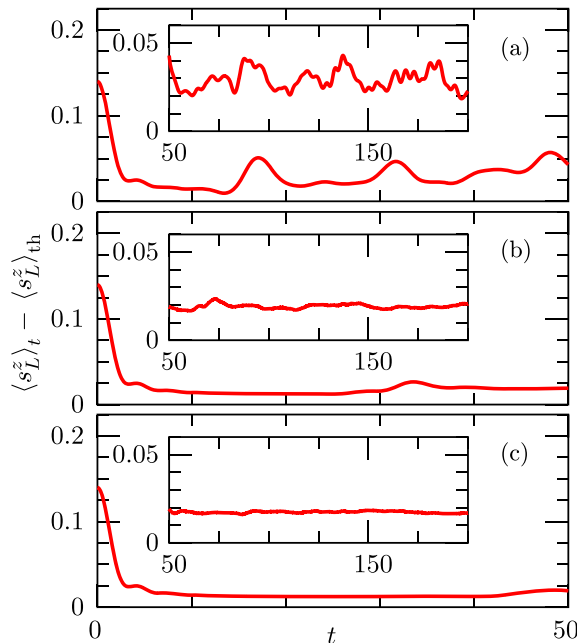


FIG. 9. Same as Fig. 5 but now for the corresponding XXZ model with $J_z = 0.3$ in Eq. (115).

Eqs. (2) and (8) [and thus in Eq. (24)] with

$$\nu = \frac{L+1}{2}, \quad (116)$$

i.e., we may imagine the impurity to be located exactly in the middle of the chain (henceforth denoted as central impurity), see also below Eqs. (8) and (42). Generalizations to even L and arbitrary inner impurities are in principle straightforward, but require more lengthy calculations and case differentiations, and will therefore only be briefly summarized at the end of this section. For the rest, the detailed calculations are largely analogous to those in the previous Sec. IV, and are therefore relegated to Appendix H.

Similarly as in Sec. IV C, the first main implication of those analytical calculations in Appendix H is that there are $L-1$ delocalized modes and one localized mode whenever $|p|$ exceeds the critical value

$$p_c := \frac{2}{\nu} = \frac{4}{L+1}, \quad (117)$$

where we utilized Eq. (116) in the last step. Furthermore, one thus can infer—similarly as in Sec. IV D—that the system exhibits no thermalization after a local quench whenever $|p| > p_c$. Quantitatively, by focusing on the most interesting regime $1/L \ll |p| \ll 1$, the counterpart of Eqs. (100) and (101) now assumes the form

$$\overline{\langle s_\alpha^z \rangle_t} - \langle s_\alpha^z \rangle_{\text{th}} = g\beta \frac{p^2 e^{-|p||\nu-\alpha|}}{16 \cosh^2(\beta/2)}. \quad (118)$$

Likewise, a strong violation of the ETH immediately follows by similar arguments as in Sec. IV D, and the concomitant signatures of localization in the system's Hamiltonian (24) are analogous to those in Sec. IV G.

The most important difference compared to the end-impurities considered in Sec. IV is that in the present case of a central impurity the critical value in Eq. (117) approaches zero for large L . In particular, a quench in the form of an arbitrarily weak central impurity thus always gives rise to non-thermalization in a sufficiently long spin-chain [see also the discussion below Eq. (101)]. We also remark that the choice $\gamma = 0$ is particularly natural in our present case [see below Eq. (8)], and implies together with Eq. (17) that the right-hand side of Eq. (118) scales as g^3 . In other words, the observable manifestations of nonthermalization are quantitatively quite weak for small g .

As an outlook we mention that for more general impurities and perturbations s_v^z in Eqs. (2) and (8) [and thus in Eq. (24)] with an arbitrary location $v \in \{1, \dots, L\}$, one finds (after similar but more involved calculations) that the critical impurity strength is given by

$$p_c = \frac{1}{\nu} + \frac{1}{L+1-\nu}, \quad (119)$$

and that the same conclusions as in the previous paragraph apply whenever $|p|$ exceeds this critical value. In particular, one readily recovers Eqs. (63) and (117) in the special cases from Eqs. (42) and (116), respectively. Moreover, p_c in Eq. (119) approaches zero whenever the impurity site ν scales with the system size L in such a way that both ν and $L-\nu$ diverge for large L . On the other hand, whenever either ν or

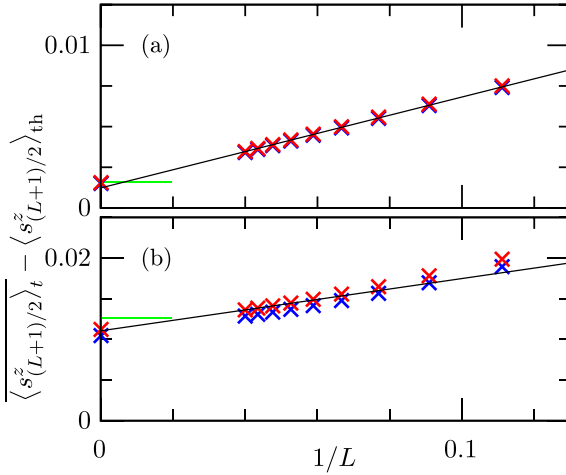


FIG. 10. Same as in Fig. 3 but now for $\nu = \alpha = (L + 1)/2$ (central impurity), $g = 0.2$ in (a), $g = 0.4$ in (b), and $L = 10001, 25, 23, \dots, 11, 9$. The green bars indicate the analytical approximation for $L \rightarrow \infty$ from Eqs. (118).

$L - \nu$ remains finite as $L \rightarrow \infty$, the critical value in Eq. (119) approaches a nonvanishing limit. Pictorially speaking, the impurity may be said to be located in the “bulk” of the spin-chain in the first case and in one of the “end-regions” in the second case.

A numerical illustration of these predictions is presented in Fig. 10 (see also Secs. IV E and V). As required at the beginning of this section, odd system sizes L have been chosen, and the values of $g = p/2$ [see Eq. (63)] are still relatively small. Overall, the main features and the discussion are largely the same as in the case of an end-impurity, see Fig. 3 and Sec. IV E, apart from one very prominent exception: We now observe absence of thermalization both in (a) and (b), in agreement with our above analytical predictions [see in particular below Eq. (118)]. Note that we have purposefully chosen in Fig. 10 even smaller values of $g = p/2$ than in Fig. 3 in order to highlight this key difference between the two cases even more strikingly. The fact that the deviations of the green bars from the leftmost blue crosses are quantitatively larger in Fig. 10 than in Fig. 3 can be traced back to the extra assumption $|p| \ll 1$ mentioned above Eq. (118). We also remark that our numerical results for even system sizes L and $\nu = \alpha = L/2$ (not shown) are found to be very similar to those in Fig. 10, i.e., the restriction to odd L and exactly centralized impurities in our above analytics indeed seems to be of minor importance.

1. Periodic boundary conditions

A further, quite minor and natural extension is to consider periodic instead of open boundary conditions. Formally, this amounts to replacing the upper summation limit $L - 1$ in Eq. (24) by L and setting $s_{L+1}^a := s_1^a$. Obviously, in such a case, the actual position ν of the impurity in Eq. (24) becomes irrelevant. Moreover, it seems reasonable to expect that the system behaves similarly as an open system with a central impurity. A confirmation of this expectation follows upon comparing the numerically exact findings in Fig. 11 with those in Fig. 10.

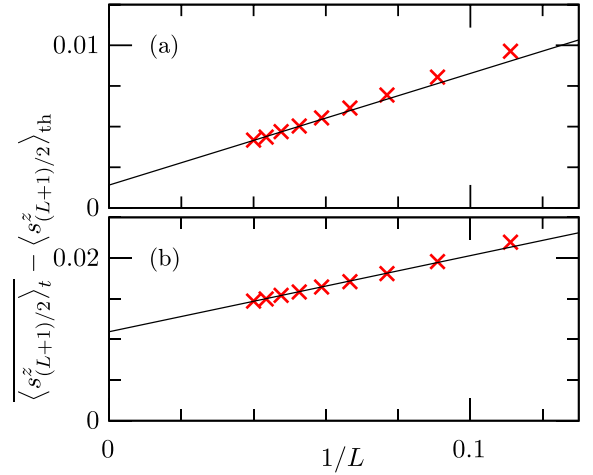


FIG. 11. Same as in Fig. 10, except that periodic instead of open boundary conditions have been employed. For more details, see the main text.

We remark that also an analytical confirmation is in principle possible by a pertinent generalization of the calculations in Secs. III and IV (see also Appendix H). We omit them here in view of the already quite considerable length of our paper as it stands. Accordingly, also the leftmost red crosses, the blue crosses, and the green bars in Fig. 10 are no longer available.

B. The XXZ model with a central impurity

As in Sec. V, we consider the XXZ model from Eq. (115), and we confine ourselves to numerical explorations. As in the previous Sec. VI A, we furthermore focus on odd chain lengths L and a central impurity according to Eq. (116).

In Fig. 12, we show the same type of numerically exact time-averaged expectation values as in Fig. 10, but now for the XXZ model (115) with $J_z = 0.3$ instead of the XX model (corresponding to $J_z = 0$), see also Fig. 7 and its discussion in Sec. V. Obviously, there is a very striking difference between

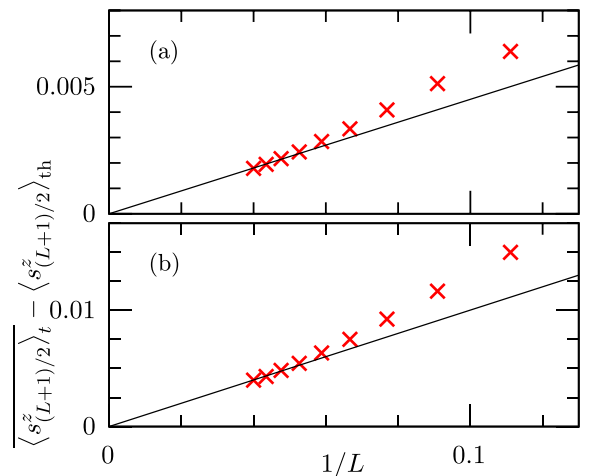


FIG. 12. Same as Fig. 10 but now for the corresponding XXZ model with $J_z = 0.3$ in Eq. (115). For more details, see the main text.

Figs. 10 and 12. While the XX model exhibits absence of thermalization in both Figs. 10(a) and 10(b), the same is no longer the case for the XXZ model both in Figs. 12(a) and 12(b) [40].

Analogous results for the same or closely related models have been reported previously, for instance, in Refs. [14,16–20]. In this sense, the example from Fig. 12 has only been included here in order to make the paper self-contained, while the observation of thermalization is in itself nothing new. Likewise, the basic physical explanation of this finding has been previously established and goes as follows: As numerically shown in Refs. [14,16–20], the well-known integrability of the XXZ model without any impurity is broken by a central impurity. More precisely speaking, it has been numerically found that the XXZ model with a central impurity satisfies the conventional (strong) ETH (see also Sec. I) and that its energy spectrum exhibits a so-called Wigner-Dyson level statistics, widely considered as a characteristic signature of “quantum chaos” and thus of nonintegrability. Similar features are also numerically seen for XXZ models with periodic boundary conditions in the presence of an impurity. Moreover, the numerics in Refs. [14,16–20] suggests that the integrability-breaking effect will persist (in the thermodynamic limit) even for arbitrary weak (but finite) impurities, and likewise for arbitrarily strong (but finite) impurities.

Incidentally, the XXZ model with open boundary conditions is well-known to remain integrable in the presence of an end-impurity [42–44], and similarly for the XX model with any (local) impurity [see below Eq. (24)]. On the other hand, the XXZ model with periodic boundary conditions is provably nonintegrable in the presence of an impurity [45]. Finally, it is reasonable to expect that a central impurity in a system with open boundary conditions results in similar properties as an impurity in a system with periodic boundary conditions. All our numerical findings are, of course, in perfect agreement with those general predictions.

VII. CONCLUSIONS

Our main finding is that already a local, and in principle arbitrarily weak quantum quench may be sufficient to prohibit a many-body system from exhibiting thermalization. Specifically, we explored the behavior of some basic local observables in XX- and XXZ-spin-chain models, initiated at thermal equilibrium (Gibbs state), and then suddenly switching on (or slightly changing) a single-spin impurity either at one of the chain’s ends or in the middle of the chain. We moreover showed that whenever a given system and observable exhibit such an absence of (re)thermalization, this observable also exhibits a strong violation of the ETH, meaning that it does not even obey the weak ETH [10]. Incidentally, this is somewhat reminiscent of the connection between the absence of thermalization after a global quench and the violation of the conventional (strong) ETH in integrable systems, which has been previously observed in numerous numerical examples (see also Sec. I).

In the case of the XX model, a fully analytical solution of the problem was possible. After employing a standard Jordan-Wigner transformation, the main achievement was to determine the eigenmodes and eigenvalues of the transformed

Hamiltonian in the presence of an impurity in the original model, see Secs. IV A, IV B, and Appendix H. We remark that somewhat similar results have been previously obtained for the transverse field Ising model with an end-impurity in Ref. [46], but that no tangible connection between the two cases can be established since they differ in too many important respects. Once these eigenmodes and eigenvalues were available, we took advantage of the recently developed general formalism from Refs. [13,26] to arrive at explicit expressions for the time-dependent expectation values. Along these lines, we analytically demonstrated the absence of thermalization in the case of an end-impurity, provided its strength exceeds some finite (nonzero) threshold value. On the other hand, in the case of an impurity in the middle of the chain, the corresponding threshold value was found to be zero, i.e., an arbitrarily weak impurity is sufficient for nonthermalization. More precisely speaking, in both cases the threshold value refers to the postquench impurity strength, while the difference between the pre- and postquench impurity strengths is even admitted to assume arbitrarily small (nonzero) values. Moreover, our analytical approximations actually become asymptotically exact when this difference becomes small.

Essentially, the absence of thermalization was found to be rooted in the appearance of a localized mode in the Jordan-Wigner transformed model. While this notion of localization—originally introduced in Ref. [39]—is of a quite formal character with respect to the original XX model in which we are actually interested, we found that its main directly observable manifestation is a localization of nonthermalization, meaning that a local quench may permanently keep the system out of equilibrium near the location of the quench, but not far away from it.

Turning to the XXZ model, analogous explorations could only be accomplished by numerical means. In the case of an end-impurity, we recovered a quite similar behavior to that of the XX model, but not anymore in the case of an impurity in the middle of the chain. As detailed in Sec. VIB, the basic reason seems to be that the XX model remains integrable in the presence of impurities at the end as well as in the middle of the chain, while the XXZ model remains integrable for end-impurities, but not anymore for impurities in the middle of the chain.

Straightforward generalizations of our analytical explorations include periodic instead of open boundary conditions (see also Sec. VIA 1), the XY instead of the XX model, or more general types of impurities and observables, to name but a few. Working out all the technical details is, however, quite a tedious task which goes beyond the scope of our present work. The same applies to a more detailed numerical exploration of the XXZ model (see Sec. VI), and likewise for the XYZ model, which may be considered as a generalization of either the XY or the XXZ model.

As explained at the end of Sec. IID, in cases where a system does *not* exhibit our present signature of nonthermalization, this is not yet sufficient to answer the question of whether or not the system actually does thermalize. Instead, a solution of this task has been worked out in our companion paper [13]. Most importantly, the occurrence of thermalization after a local quench has been rigorously established therein for the same XX model as in Secs. IV and VI, however, under

the extra condition that $g = -\gamma$ and thus $p = 0$ in Eq. (17), meaning that the prequench system in Eq. (2) exhibits an impurity, which is switched-off at time $t = 0$, resulting in an postquench system in Eq. (5) without any impurity [47]. Together with the findings of our present work, this implies that small details such as whether an impurity is switched on or off, may be of great importance with respect to the question of whether a system thermalizes or not. Moreover, to obtain truly reliable answers, a careful analytical exploration of any given specific model may be practically indispensable in general [48].

We finally note that there are also a number of similarities as well as differences between our present investigations and the topic of Hilbert space fragmentation [49]. Notable similarities are that autocorrelation functions, localization, and a strong violation of the ETH play important roles in both cases. An essential difference regarding the issue of (non)thermalization is that in the context of Hilbert space fragmentation the focus is predominantly on global quenches, or on the infinite temperature limit and some not explicitly specified nonequilibrium initial states. More detailed investigations along these lines are the subject of our ongoing work.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are openly available [50].

APPENDIX A: SAME β IN EQS. (3) AND (10)

In this Appendix, we provide a detailed justification of why β can be chosen equal in Eqs. (3) and (10) for sufficiently large L [see also the discussion above Eq. (9)].

We adopt the same definition of the system's initial state $\rho(0)$ as in Eq. (3) with an arbitrary but fixed value of β . However, instead of ρ_{can} in Eq. (10), we now consider more general canonical ensembles of the form

$$\tilde{\rho}_{\text{can}}(\tilde{\beta}) := e^{-\tilde{\beta}H} / \text{tr}\{e^{-\tilde{\beta}H}\}, \quad (\text{A1})$$

where $\tilde{\beta}$ is for the moment still arbitrary. According to textbook statistical mechanics, given a system with Hamiltonian H and some initial state $\rho(0)$, the pertinent canonical ensemble is of the general form (A1). Moreover, the value of $\tilde{\beta}$ must obviously be chosen such that the system's energy (which is a conserved quantity) is correctly reproduced. Denoting this particular $\tilde{\beta}$ value as β' , and employing the definition

$$\Delta E(\tilde{\beta}) := \text{tr}\{\rho(0)H\} - \text{tr}\{\tilde{\rho}_{\text{can}}(\tilde{\beta})H\}, \quad (\text{A2})$$

we thus require that β' satisfies

$$\Delta E(\beta') = 0. \quad (\text{A3})$$

Setting

$$\delta\beta := \beta' - \beta, \quad (\text{A4})$$

the objective in the remainder of this Appendix is to show that

$$\delta\beta = \mathcal{O}(1/L), \quad (\text{A5})$$

which is equivalent to our original claim at the beginning of this Appendix.

More precisely speaking, for our general XXZ model of the form (1), (2), (5), and (8), we will derive (A5) under the physically very reasonable extra assumption that the system's heat capacity is extensive. Moreover, for our XX model from (24), we will derive (A4) even without this extra assumption.

To begin with, let us define a set of auxiliary Hamiltonians H_r and concomitant canonical ensembles ρ_r ,

$$H_r := H_0 + r(H - H_0), \quad (\text{A6})$$

$$\rho_r := e^{-\beta H_r} / Z_r, \quad (\text{A7})$$

$$Z_r := \text{tr}\{e^{-\beta H_r}\}, \quad (\text{A8})$$

where $r \in [0, 1]$ is a parameter. Recalling the basic relations $-\frac{\partial}{\partial\beta} \ln Z_r = \text{tr}\{\rho_r H_r\}$ and $H = H_0 + gV$ [see Eq. (5)], we can conclude from Eq. (A2) that

$$\Delta E(\beta) = g \text{tr}\{\rho(0)V\} + \frac{\partial}{\partial\beta} \ln \frac{Z_1}{Z_0}. \quad (\text{A9})$$

Furthermore, by exploiting Eqs. (C.9) and (C.11) in the supplemental material of Ref. [11] and the cyclic invariance of the trace, one can infer the relation

$$\ln \frac{Z_1}{Z_0} = -g\beta \int_0^1 dr \text{tr}\{\rho_r V\}, \quad (\text{A10})$$

yielding with (A9) the result

$$\Delta E(\beta) = g[C_1(\beta) - C_2(\beta) - \beta C_3(\beta)], \quad (\text{A11})$$

$$C_1(\beta) := \text{tr}\{\rho(0)V\}, \quad (\text{A12})$$

$$C_2(\beta) := \int_0^1 dr \text{tr}\{\rho_r V\}, \quad (\text{A13})$$

$$C_3(\beta) := \int_0^1 dr \frac{\partial}{\partial\beta} \text{tr}\{\rho_r V\}. \quad (\text{A14})$$

Observing that $|\text{tr}\{\rho_r V\}| \leq \|V\|_{\text{op}}$ for all r (where $\|\cdot\|_{\text{op}}$ denotes the operator norm, see also below Eq. (16)), and utilizing the abbreviations

$$v := \|V\|_{\text{op}}, \quad (\text{A15})$$

$$D := \frac{1}{v} \max_{0 \leq r \leq 1} \left| \frac{\partial}{\partial\beta} \text{tr}\{\rho_r V\} \right|, \quad (\text{A16})$$

we can upper bound the modulus of the three quantities in Eqs. (A12)–(A14) and then conclude with Eq. (A11) that

$$|\Delta E(\beta)| \leq |g|v(2 + |\beta|D). \quad (\text{A17})$$

Next, we can infer from (A3) that

$$\Delta E(\beta) = \int_{\beta'}^{\beta} d\tilde{\beta} W(\tilde{\beta}), \quad (\text{A18})$$

$$W(\tilde{\beta}) := \frac{\partial}{\partial \tilde{\beta}} \Delta E(\tilde{\beta}), \quad (\text{A19})$$

and with (A2) that

$$W(\tilde{\beta}) = -\frac{\partial}{\partial \tilde{\beta}} \text{tr}\{\tilde{\rho}_{\text{can}}(\tilde{\beta}) H\}. \quad (\text{A20})$$

Invoking (A4), we can evaluate (A18) by the mean-value theorem and introduce the result into (A17), implying

$$|\delta\beta| \leq \frac{|g|v(2 + |\beta|D)}{|W(\beta_m)|}, \quad (\text{A21})$$

for some β_m with the property $\beta - |\delta\beta| \leq \beta_m \leq \beta + |\delta\beta|$.

1. Evaluation of D and $W(\beta_m)$

Let us first remark that the derivation of (A21) is still valid for entirely general Hamiltonians H and H_0 . Furthermore, our final result (A5) follows immediately from (A21) under the following three conditions: (i) v in (A15) remains bounded for $L \rightarrow \infty$, (ii) D in (A16) remains bounded for $L \rightarrow \infty$, and (iii) $|W(\beta_m)|$ in (A19) grows asymptotically linearly with L .

Condition (i) is trivially fulfilled for any local operator V . In particular, for our standard example from Eq. (8), one finds that

$$v = \|s_v^z\|_{\text{op}} = 1/2, \quad (\text{A22})$$

see also below Eq. (16). Conditions (ii) and (iii) are in general more difficult to verify mathematically, but physically speaking it seems very reasonable to expect that they will be fulfilled in many cases. For instance, the quantity $W(\beta_m)$ in Eq. (A20) can be immediately related to the system's heat capacity. Hence, it is expected to be an extensive quantity in many cases, including our XXZ model of the form (1), (2), (5), and (8). Similarly, (ii) is expected to hold as long as there is no (first-order) phase transition at inverse temperature β and with an order parameter related to V , which again can be excluded for our present one-dimensional models.

Moreover, in cases where the Hamiltonian H_r is given by a sum of local operators of the general structure $H_r = \sum_l h_l$ (which applies, for instance, for our present XXZ model), one readily verifies that

$$\frac{\partial}{\partial \beta} \text{tr}\{\rho_r V\} = -\sum_l G(V, h_l), \quad (\text{A23})$$

where

$$G(A, B) := \text{tr}\{\rho_r AB\} - \text{tr}\{\rho_r A\} - \text{tr}\{\rho_r B\} \quad (\text{A24})$$

is the correlation of the operators A and B . For the canonical ensembles ρ_r and local perturbations V we are considering here, one can furthermore show that the correlations $G(V, h_l)$ exhibit a so-called cluster decomposition property [51], from which one can deduce that the sum in (A23) can be upper bounded (in modulus) by a finite value when $L \rightarrow \infty$. Note that this argument applies separately to any given parameter value r , hence it also applies to that r value which maximises the right-hand side of (A16) in the limit $L \rightarrow \infty$. Incidentally, one might think that similar arguments may also be applicable with respect to the above condition (iii). The problem is that,

in contrast to (ii), it is necessary to establish some suitable kind of *lower* bound in order to guarantee (iii).

Finally, we provide a more rigorous justification of (ii) and (iii) for the XX model within the setup considered in Secs. III and VI A. Regarding (ii), we can identify $\text{tr}\{\rho_r V\}$ with the left-hand side of Eq. (G1) with $\alpha = v$, while the r dependence of $\text{tr}\{\rho_r V\}$ is buried in the quantities U_{kv} and E_k on the right-hand side of Eq. (G1). Utilizing $\frac{d}{dx} \tanh(x) = 1/\cosh^2(x)$, one thus obtains

$$\frac{\partial}{\partial \beta} \text{tr}\{\rho_r V\} = -\frac{1}{4} \sum_{k=1}^L |U_{kv}|^2 \frac{E_k}{\cosh^2(\beta E_k/2)}. \quad (\text{A25})$$

Furthermore, one can readily infer from the discussions in Sec. IV B and Appendix H that

$$|E_k| \leq h(p) \quad (\text{A26})$$

for all admissible k and L , where $h(p)$ is an L -independent function with $h(0) = 1$ and $h(p) \approx \mathcal{O}(|p|)$ for $p \gg 1$. Recalling that $\sum_{k=1}^L |U_{kl}|^2 = 1$ (see below Eq. (39)) and that $\cosh(x) \geq 1$, we thus can conclude that

$$\left| \frac{\partial}{\partial \beta} \text{tr}\{\rho_r V\} \right| \leq \frac{h(p)}{4} \quad (\text{A27})$$

independent of r , and with (A17) that

$$D \leq \frac{h(p)}{4} \quad (\text{A28})$$

independent of L , i.e., condition (ii) is fulfilled.

Turning to (iii), our first observation is that the pertinent quantity $|W(\beta)|$ can be identified with $\frac{\partial^2}{\partial \beta^2} \ln Z_1$ [see also below Eq. (A8)]. Our next observation is that $\ln Z_1$ can be readily evaluated by means of the eigenbasis $|\vec{b}\rangle$ of H as specified in and around Eqs. (30)–(32) and recalling that $H_1 = H$ according to Eq. (A6). The detailed calculations are straightforward and very similar as, for instance, those in Appendix B.1 of Ref. [13]. Along these lines, one finally arrives at the result

$$|W(\beta_m)| = \sum_{l=1}^L \frac{E_l^2}{4 \cosh^2(\beta_m E_l/2)}. \quad (\text{A29})$$

Upon utilizing (A26), we thus can conclude that

$$|W(\beta_m)| \geq \frac{1}{4 \cosh^2(\beta_m h(p)/2)} \sum_{l=1}^L E_l^2. \quad (\text{A30})$$

Denoting by N_L the number of indices $l \in \{1, \dots, L\}$ with the property $|E_l| \geq \frac{1}{2}$ it follows that

$$|W(\beta_m)| \geq \frac{N_L}{16 \cosh^2(\beta_m h(p)/2)}. \quad (\text{A31})$$

Focusing on energies E_l of the type discussed in Sec. IV B 1 and Appendix H, one readily sees that for large L at least half of them satisfy the condition $|E_l| \geq \frac{1}{2}$, i.e., $N_L \geq L/2$. Together with Eqs. (A21), (A22), (A28), and (A31), we thus can conclude that

$$|\delta\beta| \leq \frac{4|g|(8 + |\beta|h(p)) \cosh^2(\beta_m h(p)/2)}{L}. \quad (\text{A32})$$

The remaining task is to show that the right-hand side approaches zero for $L \rightarrow \infty$. Recalling that g , β , and p are

considered as arbitrary but fixed, it is thus sufficient that β_m remains finite for $L \rightarrow \infty$. According to (A4) and the specification of β_m below (A21), the latter in turn is guaranteed if the solution β' of the equation (A3) remains bounded for $L \rightarrow \infty$. It seems reasonable to expect that the latter, very weak condition can safely be taken for granted in most cases of physical interest. Indeed, an unlimited growth of β' essentially corresponds to the zero temperature limit and would mean that the system assumes an extremely low energy after a local quantum quench (and likewise if $\beta' \rightarrow -\infty$). Tacitly ignoring such cases, the numerator in (A32) stays bounded for $L \rightarrow \infty$, and we recover our final result (A5). [Incidentally, once we know that $\delta\beta$ is small, we can approximate β_m in (A32) by β according to the specification of β_m below Eq. (A21).]

APPENDIX B: MONOTONICITY

The objective is to show that for any $n \in \mathbb{N}$, the function

$$g(x) := \sin(x) \cot(nx) \quad (\text{B1})$$

is strictly monotonically decreasing for all $x \in (0, \pi)$ with $nx/\pi \notin \mathbb{Z}$. [Note that $g(x)$ is not defined (exhibits poles) for $nx/\pi \in \mathbb{Z}$.] Since $\cos(x)$ is monotonically decreasing for all $x \in (0, \pi)$, it readily follows that also the function

$$f(x) := \cos(x) + \sin(x) \cot(Lx) \quad (\text{B2})$$

is strictly monotonically decreasing for all $x \in (0, \pi)$ with $Lx/\pi \notin \mathbb{Z}$, as claimed in item (iii) above Eq. (63).

We therefore rewrite the derivative of $g(x)$ as

$$g'(x) = -h(x)/\sin^2(nx), \quad (\text{B3})$$

$$\begin{aligned} h(x) &:= -\cos(x) \cos(nx) \sin(nx) + n \sin(x) \\ &= n \sin(x) - \cos(x) \sin(2nx)/2. \end{aligned} \quad (\text{B4})$$

It is thus sufficient to show that $h(x) > 0$ for all $x \in (0, \pi)$. Observing that $h(\pi - x) = h(x)$, it is furthermore sufficient to focus on $x \in (0, \pi/2]$. Since $|\cos(x) \sin(2nx)/2| < 1/2$ for all those x , it readily follows that $h(x) > 0$ for all $x \in (0, \pi/2]$ with the property $\sin(x) \geq 1/2n$. We are thus left with those $x \in (0, \pi/2]$ with the property $\sin(x) < 1/2n$. Since $\cos(x) < 1$ for all those x , it is sufficient to show that

$$2n \sin(x) \geq \sin(2nx) \quad (\text{B5})$$

for all $x \in (0, \pi/2]$ with $\sin(x) < 1/2n$.

Our next observation is that $\cos(\alpha y) \geq \cos(y)$ for all $y \in [0, \pi]$ and arbitrary $\alpha \in (0, 1]$, implying

$$\frac{\sin(\alpha y)}{\alpha} = \int_0^y dx \cos(\alpha x) \geq \int_0^y dy \cos(x) = \sin(y). \quad (\text{B6})$$

Choosing $\alpha = 1/2n$ and $y = x/\alpha = 2nx$ it follows that Eq. (B5) is fulfilled for all $x \in [0, \pi/2n]$. Observing that the solution $x \in (0, \pi/2]$ of $\sin(x) = 1/2n$ satisfies $x \leq \pi/2n$ for any $n \in \mathbb{N}$, we can conclude that, indeed, Eq. (B5) is fulfilled for all $x \in (0, \pi/2]$ with $\sin(x) < 1/2n$.

APPENDIX C: DERIVATION OF EQ. (83)

Focusing first on $p = 1$, our goal is to find L solutions r_k of Eq. (78) under the extra constraint $r_k \in (-\pi, 0)$, see Eqs. (60), (64), and below (74). Introducing

$$x_k := -r_k, \quad (\text{C1})$$

$$y_k := \frac{\pi k}{L+1} + \frac{L}{L+1} x_k, \quad (\text{C2})$$

it follows that $x_k \in (0, \pi)$ and $y_k \in (0, 2\pi)$ for all $k \in \{1, \dots, L\}$, while Eq. (78) together with Eq. (63) can be rewritten as

$$\sin(x_k) = \sin(y_k). \quad (\text{C3})$$

One readily sees that this equation admits at most two possible solutions under the extra constraints $x_k \in (0, \pi)$ and $y_k \in (0, 2\pi)$, namely, (i) $x_k = y_k$ and (ii) $x_k - \pi/2 = \pi/2 - y_k$. In the case (i), one can conclude with Eq. (C2) that $x_k = k\pi$, thus violating one of the constraints. Likewise, in the case (ii) one recovers with Eqs. (C1) and (C2), the result from Eq. (83).

Turning to the case $p = -1$, one recovers again Eq. (C3) if one defines

$$x_k := r_k, \quad (\text{C4})$$

$$y_k := \frac{\pi k}{L+1} - \frac{L}{L+1} x_k, \quad (\text{C5})$$

satisfying $x_k \in (0, \pi)$ and $y_k \in (-\pi, \pi)$, and implying again the two possible solutions (i) and (ii). However now, (i) implies Eq. (83), while (ii) violates the constraints.

APPENDIX D: DERIVATION OF EQ. (93)

Our objective is to show that Eq. (93) amounts to an approximation whose relative error decreases as $1/L$ for $L \rightarrow \infty$. In particular, we always take for granted that L is large. More precisely speaking [see around Eq. (93)], the quantity κ_k in Eq. (93) may either be defined via Eq. (68) with $k \in \{1, \dots, L-1\}$ (corresponding to the case $|p| > p_c$) or via Eq. (77) with $k \in \{1, \dots, L\}$ (corresponding to the case $|p| < p_c$).

We first consider the case $|p| > p_c$. Since $\sin(0) = 0$, we can replace the lower summation limit $l = 1$ in Eq. (68) by $l = 0$. Observing $\sin^2(x) = [1 - \cos(2x)]/2$, we thus can infer from Eq. (68) that

$$\kappa_k^2 = [L+1-R]/2, \quad (\text{D1})$$

$$R := \sum_{l=0}^L \cos(\psi l), \quad (\text{D2})$$

$$\psi := 2\varphi_k, \quad (\text{D3})$$

where φ_k is defined in Eq. (64). Since $\varphi_k \in (0, \pi)$ for all k , see Eq. (61), it follows that $e^{i\psi} \neq 1$ and thus

$$R = \text{Re}(Q), \quad (\text{D4})$$

$$Q := \sum_{l=0}^L e^{i\psi l} = \frac{1 - e^{i\psi(L+1)}}{1 - e^{i\psi}}, \quad (\text{D5})$$

where $\chi := (L + 1)\psi$. Together with Eqs. (D3) and (64), it follows that $\chi = \psi + 2(\pi k + r_k)$. As far as the quantity $e^{i\chi}$ in Eq. (D5) is concerned, we therefore can equally well employ the definition

$$\chi := \psi + 2r_k. \quad (\text{D6})$$

Let us first focus on k values with $k \ll L$, say $k/L \leq \epsilon$ with some small $\epsilon > 0$. It follows with Eqs. (64) and (71) that ψ in Eq. (D3) as well as χ in Eq. (D6) are small quantities (of order ϵ or smaller). Hence Q in Eq. (D5) can be approximated as

$$Q \simeq \frac{\chi}{\psi} = 1 + \frac{r_k}{\varphi_k} = 1 + \frac{Lr_k}{\pi k + r_k}, \quad (\text{D7})$$

where we used Eqs. (D3) and (D6) in the second step, and Eq. (64) in the last step. Observing Eq. (71), it follows that the last term in Eq. (D7) can be approximated by $1/(p - p_c + 1/L)$ and thus by $1/(p - p_c)$ for sufficiently large L . Together with (D4) and (D7), this yields $R \simeq 1 + 1/(p - p_c)$. Rewriting Eq. (D1) as

$$\kappa_k^2 = \frac{L}{2}(1 + a), \quad (\text{D8})$$

$$a := \frac{1 - R}{L}, \quad (\text{D9})$$

we thus recover the approximation (93) with a relative error a which decreases as $1/L$ for large L . Analogous considerations apply for all k with $\bar{k}/L \leq \epsilon$, where $\bar{k} := L - k$. Next we turn to the remaining k values with the properties $k/L > \epsilon$ and $\bar{k}/L > \epsilon$. Taking into account Eqs. (64) and (65) it follows that ψ from (D3) must be larger than $\tilde{\epsilon} := \pi\epsilon - \pi/L$ and smaller than $2\pi - \tilde{\epsilon}$. For sufficiently large L , we thus can conclude that $\psi \geq \epsilon$ and $\psi < 2\pi - \epsilon$. Since ϵ is small it follows that $|1 - e^{i\psi}|$ can be lower bounded by ϵ apart from corrections of order ϵ^2 . Hence, $|Q|$ in Eq. (D5) and $|R|$ in Eq. (D4) can be upper bounded by $2/\epsilon$. Together with Eqs. (D8) and (D9), this yield once again the approximation (93) with a relative error $a \propto 1/L$.

Finally, we turn to the case $|p| < p_c$ (see also the first paragraph). One readily sees that essentially the same line of reasoning as before can be employed, except that one now has to work with Eqs. (74), (80), and (81) instead of Eqs. (64), (71), and (72), respectively. Moreover, in the special case $p = 0$, one finds the *exact* result $\kappa_k = \sqrt{(L + 1)/2}$ (for arbitrary L) as an improvement of the large- L approximation (93).

APPENDIX E: STRONG VIOLATION OF THE ETH FOR $|p| > p_c$

In this Appendix, we provide a direct proof of the strong violation of the ETH for $|p| > p_c$, as announced at the end of Sec. IV D 2.

To begin with, we recall [7] that the ETH essentially means that the diagonal matrix elements $\langle n|A|n \rangle$ of any (local) observable A must be similar for energy eigenstates $|n \rangle$ with similar eigenvalues $\mathcal{E}_n$, see also in and around Eqs. (21) and (22). More precisely speaking [7], it is sufficient to focus on large system sizes, and the variations of $\langle n|A|n \rangle$ must be negligible as long as the differences of the energies $\mathcal{E}_n$ are small compared to the typically extensive energy scale of the

system itself. The conventional (or strong) ETH requires that *all* eigenstates $|n \rangle$ (with energies $\mathcal{E}_n$ not too close to the edges of the spectrum) exhibit this property [7]. On the other hand, a few exceptional eigenstates are still admitted in the case of the weak ETH (wETH) [10], but their fraction is required to approach zero with increasing system size.

As already noted in brackets below Eq. (32), instead of the eigenvectors $|n \rangle$ and eigenvalues $\mathcal{E}_n$ of H as introduced above Eq. (21), we can equally well work with the eigenvectors $|\vec{b} \rangle$ and eigenstates $E(\vec{b})$ from Eqs. (31) and (32), respectively. Taking into account Eqs. (30), (33), (34) and the fermionic anticommutation relations for $f_k^\dagger$ and f_k , a straightforward calculation then yields for the diagonal matrix elements of the observable $A = s_\alpha^z$ [see also Eq. (11)] the result

$$\langle \vec{b} | s_\alpha^z | \vec{b} \rangle = \left(\sum_{k=1}^L b_k |U_{k\alpha}|^2 \right) - 1/2, \quad (\text{E1})$$

where b_k are the binary components of $\vec{b}$ [see above Eq. (30)].

Let us choose an arbitrary but fixed eigenstate $|\vec{b} \rangle$ and define a second eigenstate $|\vec{b}' \rangle$ with $b'_k = b_k$ for all $k \in \{1, \dots, L - 1\}$ and $b'_L \neq b_L$ (i.e., $b'_L = 1$ if $b_L = 0$ and vice versa). Hence, the difference of the two energies is, according to Eq. (32),

$$|E(\vec{b}') - E(\vec{b})| = |E_L|. \quad (\text{E2})$$

Focusing on the case $|p| > p_c$ and exploiting the large- L approximation (88), it follows that

$$|E(\vec{b}') - E(\vec{b})| = |p + 1/p|/2. \quad (\text{E3})$$

Likewise, the difference of the corresponding diagonal matrix elements is, according to Eq. (E1),

$$|\langle \vec{b}' | s_\alpha^z | \vec{b}' \rangle - \langle \vec{b} | s_\alpha^z | \vec{b} \rangle| = |U_{L\alpha}|^2 = (1 - 1/p^2)(1/p)^{2\bar{\alpha}}, \quad (\text{E4})$$

where we exploited Eqs. (89) and (90) in the last step. Hence, the difference in Eq. (E4) is non-negligible compared to the two possible measurement outcomes $\pm 1/2$ of the observable $A = s_\alpha^z$ [21], for instance, if $\alpha = L$ and $|p|$ is not too close to $p_c \simeq 1$. Likewise, the energy difference in Eq. (E3) might appear not to be really small. However, as said in the second paragraph of the present Appendix, it is not this energy difference itself that counts, but rather the difference is required to grow not too fast (usually sublinearly) with the system size L , which is clearly the case.

In summary, for every given energy eigenstate, there exists a “partner state” which is energetically close while the diagonal matrix elements are notably different at least for one local observable $A = s_L^z$. It follows that both the ETH and the wETH are violated, i.e., we recover the announced strong violation of the ETH for $|p| > p_c$.

APPENDIX F: NUMERICAL EVALUATION OF THE EXACT QUENCH DYNAMICS

This Appendix provides the details of our optimized numerical treatment of long XX-chains, as announced in Sec. IV E.

As a slightly more general starting point, we consider cases where H in Eq. (5) as well as H_0 in Eq. (2) can be written in the form

$$H = \sum_{k,l=1}^L B_{kl} c_k^\dagger c_l, \quad (\text{F1})$$

$$H_0 = \sum_{k,l=1}^L \tilde{B}_{kl} c_k^\dagger c_l, \quad (\text{F2})$$

with fermionic creation and annihilation operators $c_l^\dagger$ and c_l , respectively, and arbitrary coefficients B_{kl} and $\tilde{B}_{kl}$ apart from the hermiticity conditions $B_{lk} = B_{kl}^*$ and $\tilde{B}_{lk} = \tilde{B}_{kl}^*$. In particular, XX models with Hamiltonians H as in Eq. (24) can be recast by means of a Jordan-Wigner transformation into the form (26) and thus (F1), and likewise for H_0 . Similarly as in Eqs. (27) and (28), there furthermore must exist unitary $L \times L$ matrices U and $\tilde{U}$ with entries U_{kl} and $\tilde{U}_{kl}$, respectively, so that

$$H = \sum_{k=1}^L E_k f_k^\dagger f_k, \quad (\text{F3})$$

$$H_0 = \sum_{k=1}^L \tilde{E}_k \tilde{f}_k^\dagger \tilde{f}_k, \quad (\text{F4})$$

where

$$f_k := \sum_{l=1}^L U_{kl} c_l, \quad (\text{F5})$$

$$\tilde{f}_k := \sum_{l=1}^L \tilde{U}_{kl} c_l, \quad (\text{F6})$$

and their adjoints $f_k^\dagger$ and $\tilde{f}_k^\dagger$ are again fermionic annihilation and creation operators. In other words, U is the unitary matrix diagonalizing the matrix B with entries B_{kl} , while $\tilde{U}$ diagonalizes $\tilde{B}$ with entries $\tilde{B}_{kl}$. Inverting Eq. (F6) and introducing the resulting expression into Eq. (F5) yields

$$f_k = \sum_{l=1}^L S_{kl} \tilde{f}_l, \quad (\text{F7})$$

$$S_{kl} := \sum_{m=1}^L U_{km} \tilde{U}_{lm}^*. \quad (\text{F8})$$

Adopting the same definition as in Eq. (13),

$$A(t) := e^{iHt} A e^{-iHt}, \quad (\text{F9})$$

but now for arbitrary (not necessarily Hermitian) operators A , and utilizing Eq. (B14) from [13], which takes the form

$$f_k(t) = e^{-iE_k t} f_k \quad (\text{F10})$$

in our present notation, we can conclude that

$$c_l(t) = \sum_{k=1}^L U_{kl}^* f_k(t) \quad (\text{F11})$$

$$= \sum_{k=1}^L U_{kl}^* e^{-iE_k t} \sum_{m=1}^L S_{km} \tilde{f}_m. \quad (\text{F12})$$

Exploiting Eq. (F9) it follows that $[c_l^\dagger c_l](t) = [c_l(t)]^\dagger c_l(t)$, and together with Eq. (12) that

$$\langle c_l^\dagger c_l \rangle_t = \sum_{j,k=1}^L U_{jl} U_{kl}^* e^{i(E_j - E_k)t} T_{jk}, \quad (\text{F13})$$

$$T_{jk} := \sum_{m,n=1}^L S_{jm}^* S_{kn} p_{mn}, \quad (\text{F14})$$

$$p_{mn} := \text{tr}[\rho(0) \tilde{f}_m^\dagger \tilde{f}_n]. \quad (\text{F15})$$

To further evaluate the right-hand side of Eq. (F15), we focus on our specific initial conditions from Eq. (3). By exploiting (F4), one thus finds after a straightforward calculation (see e.g. Eqs. (B21)–(B29) in Ref. [13] for the details)

$$p_{mn} = \frac{1}{1 + e^{\beta E_m}} \delta_{mn}. \quad (\text{F16})$$

Hence, Eq. (F14) simplifies to

$$T_{jk} = \sum_{n=1}^L \frac{S_{jn}^* S_{kn}}{1 + e^{\beta E_n}}, \quad (\text{F17})$$

and with Eqs. (33), we arrive at our final result

$$\langle s_l^z \rangle_t = \langle c_l^\dagger c_l \rangle_t - 1/2, \quad (\text{F18})$$

which can be evaluated by employing Eqs. (F8), (F13), and (F17).

Overall, the numerical effort to evaluate the expectation value (F18) along these lines only grows algebraically with the system size L , while it grows exponentially when employing standard methods based on a direct diagonalization of the Hamiltonian H in Eq. (24), see also Sec. IV E.

APPENDIX G: EVALUATION OF $\langle s_\alpha^z \rangle_{\text{th}}$

The thermal expectation value in Eq. (9) for our standard observables $A = s_\alpha^z$ [see Eq. (11)] and Hamiltonians H [see Eq. (24)] can be analytically evaluated without any approximation, as shown in Ref. [13] [see Eq. (B41) therein], yielding

$$\langle s_\alpha^z \rangle_{\text{th}} = -\frac{1}{2} \sum_{k=1}^L |U_{k\alpha}|^2 \tanh(\beta E_k/2). \quad (\text{G1})$$

We recall that Eq. (G1) must be an odd of function p [see below Eq. (17)]. Furthermore, Eq. (G1) is obviously an odd function of β .

In order to obtain more detailed quantitative results, we henceforth focus—as in Sec. IV of the main paper—on impurities at the right chain-end [i.e., with $v = L$, see in and around Eq. (42)]. Hence, we can exploit our results for U_{kl} and E_k from Sec. IV B.

Let us first address the case $|p| < p_c$. Exploiting Eqs. (64), (66), and (67), we obtain

$$U_{k\alpha} = \kappa^{-1} \sin(\varphi_k \alpha), \quad (\text{G2})$$

$$E_k = \cos(\varphi_k). \quad (\text{G3})$$

Since the $U_{k\alpha}$ are the elements of a unitary matrix [see below Eq. (26)], we can conclude with Eq. (G2) that

$$\sum_{k=1}^L \kappa_k^{-2} \sin(\varphi_k m) \sin(\varphi_k n) = \sum_{k=1}^L U_{km}^* U_{kn} = \delta_{mn} \quad (\text{G4})$$

for all $m, n \in \{1, \dots, L\}$.

To make further progress, we adopt the same assumption as in Eq. (103) and approximate the tanh function in Eq. (G1) by its leading order approximation in β . Together with Eqs. (G2) and (G3), we thus obtain

$$\langle s_\alpha^z \rangle_{\text{th}} = -\frac{\beta}{4} \sum_{k=1}^L \kappa_k^{-2} \sin^2(\varphi_k \alpha) \cos(\varphi_k). \quad (\text{G5})$$

Observing that $\sin(x) \cos(y) = [\sin(x+y) + \sin(x-y)]/2$, it follows that

$$\langle s_\alpha^z \rangle_{\text{th}} = -\frac{\beta}{8} (S_\alpha^+ + S_\alpha^-), \quad (\text{G6})$$

$$S_\alpha^\pm := \sum_{k=1}^L \kappa_k^{-2} \sin(\varphi_k \alpha) \sin(\varphi_k (\alpha \pm 1)). \quad (\text{G7})$$

With Eq. (G2) we can conclude that $S_\alpha^- = 0$ for all $\alpha \in \{2, \dots, L\}$. For $\alpha = 1$, the same follows immediately from Eq. (G7). Likewise, one sees that $S_\alpha^+ = 0$ for all $\alpha \in \{1, \dots, L-1\}$, yielding

$$\langle s_\alpha^z \rangle_{\text{th}} = -\delta_{\alpha L} \frac{\beta}{8} S, \quad (\text{G8})$$

$$S := \sum_{k=1}^L \kappa_k^{-2} \sin(\varphi_k L) \sin(\varphi_k (L+1)). \quad (\text{G9})$$

Finally, we recall that all the φ_k are solutions of Eqs. (61) and (62), i.e., $\sin(\varphi_k (L+1)) = p \sin(\varphi_k L)$, implying

$$S := p \sum_{k=1}^L \kappa_k^{-2} \sin^2(\varphi_k L) = p, \quad (\text{G10})$$

where we exploited Eq. (G4) in the last step. With Eq. (G8), we thus obtain in leading order β the result

$$\langle s_\alpha^z \rangle_{\text{th}} = -\delta_{\alpha L} \frac{\beta p}{8}. \quad (\text{G11})$$

Most importantly, Eq. (G11) tells us that, in leading order β , only the spin at the right chain-end $\alpha = L$ is affected by an impurity at the right chain-end $v = L$. Furthermore, Eq. (G11) is in agreement with the prediction below Eq. (G1) that $\langle s_\alpha^z \rangle_{\text{th}}$ must be an odd function of p and of β . Moreover, it follows that the neglected corrections on the right-hand side of Eq. (G11) must be (at least) of order β^3 . On the other hand, we did *not* assume that p is a small quantity, i.e., the linearity of Eq. (G11) in p applies for all $|p| < p_c$ (at least in leading order β).

From the structure of Eqs. (G1) and (G5)–(G10) it is quite obvious that keeping higher and higher powers of β in the expansion of the tanh function in Eq. (G1) has two main effects. (i) On the right-hand side of Eq. (G11) there will appear additional summands with higher and higher (odd) powers of β , each multiplied with an (odd) polynomial of p of the same order as β . (ii) Analogously to the Kronecker

δ in Eq. (G11), the coefficients of these polynomials will depend on α such that more and more spins near the right chain-end assume nonvanishing values (which, however, are expected to still decrease with increasing distance from the chain-end). Working out the details is straightforward but not further pursued here.

Next we turn to the case $|p| > p_c$. The salient point consists in the following observation: If we do *not* replace φ by $i\varphi$, as it is done in case B below Eq. (56), then those φ 's will become purely imaginary quantities, but for the rest they still satisfy exactly the same equations as in case A, most importantly Eqs. (48), (49), and (51). As a consequence, also Eqs. (G2)–(G11) can be taken over, except that the first factor $\sin(\varphi_k m)$ in Eq. (G4) has to be replaced by its complex conjugate, and analogously in Eqs. (G5), (G7), (G9), and (G10).

Altogether, the main result (G11) is thus found to be valid both for $|p| < p_c$ and $|p| > p_c$. The validity in the case $|p| = p_c$ follows by continuity. In conclusion, Eq. (G11) as well as the discussion below (G11) is valid for arbitrary p . Since the left-hand side of Eq. (G11) is bounded in modulus by $1/2$ it follows that the neglected higher order corrections on the right-hand side will become more and more important with increasing values of p . In particular, the same (odd) power series in β mentioned below Eq. (G11) is expected to apply (and converge) for arbitrary p . Hence, the qualitative properties of the thermal expectation values on the left-hand side of Eq. (G11) do *not* exhibit any kind of “transition” when $|p|$ crosses the critical value p_c .

Incidentally, the result (G11) and its generalization to arbitrary v can be obtained even more easily by exploiting Eq. (15) for $t = 0$ and the small- β asymptotics of Eqs. (35)–(37), yielding

$$\langle A \rangle_0 - \langle A \rangle_{\text{th}} = \frac{g\beta}{4} \left| \sum_{k=1}^L U_{kv}^* U_{k\alpha} \right|^2 = \frac{g\beta}{4} \delta_{\alpha v}. \quad (\text{G12})$$

Apart from the small- β approximation [see also Eq. (103)], this result becomes asymptotically exact for small g according to the discussion below Eq. (16). In view of Eqs. (3) and (4), the first term $\langle A \rangle_0$ in Eq. (G12) is the thermal expectation value for the prequench Hamiltonian (2) with an arbitrary but fixed value of γ . Observing Eqs. (5), (9), and (10), the left-hand side of Eq. (G12) can be identified with the (negative) change of the thermal expectation value when increasing γ in Eq. (2) by g . According to Eqs. (17) and (24) we thus can increase p by means of many small steps in g , and add up the corresponding small (negative) changes of the thermal expectation values on the left-hand side of Eq. (G12). Moreover, from the symmetry properties below Eq. (G1), we can conclude that the thermal expectation value vanishes for $\gamma = 0$. Starting with $\gamma = 0$ and letting the step size go to zero one thus obtains

$$\langle s_\alpha^z \rangle_{\text{th}} = -\delta_{\alpha v} \frac{\beta p}{8}. \quad (\text{G13})$$

[The extra factor of $1/2$ in (G13) compared to Eq. (G12) has its origin in the factor 2 on the right-hand side of Eq. (17).] While this way of deriving the leading-order-in- β behavior is even easier than in our previous calculations, the generalization to higher orders in β turns out to be more involved.

APPENDIX H: ANALYTICAL SOLUTION FOR A CENTRAL IMPURITY

For the central impurities from Eq. (115), we can rewrite Eq. (40) as

$$a_{l+1} + a_{l-1} = 2Ea_l \quad \text{for } l \in \{2, \dots, L-1\} \setminus \{v\}, \quad (\text{H1})$$

$$a_{v+1} + a_{v-1} = (2E - p)a_v, \quad (\text{H2})$$

$$a_2 = 2Ea_1, \quad (\text{H3})$$

$$a_{L-1} = 2Ea_L. \quad (\text{H4})$$

Similarly as in Eqs. (46)–(49), this suggest the ansatz

$$a_l = \alpha_l \quad \text{for } l \in \{1, \dots, v-1\}, \quad (\text{H5})$$

$$a_l = \beta_l \quad \text{for } l \in \{v+1, \dots, L\}, \quad (\text{H6})$$

$$\alpha_l := \sin(\varphi l) \quad \text{for all } l \in \mathbb{Z}, \quad (\text{H7})$$

$$\beta_l := B \sin(\varphi(L+1-l)) \quad \text{for all } l \in \mathbb{Z}, \quad (\text{H8})$$

involving three, generally complex valued parameters φ , B , and a_v . Observing that

$$\alpha_{l+1} + \alpha_{l-1} = 2 \cos(\varphi) \alpha_l \quad \text{for all } l \in \mathbb{Z}, \quad (\text{H9})$$

$$\beta_{l+1} + \beta_{l-1} = 2 \cos(\varphi) \beta_l \quad \text{for all } l \in \mathbb{Z}, \quad (\text{H10})$$

it follows that Eqs. (H5) and (H6) indeed solve Eq. (H1) for all $l = 2, \dots, v-2$ and $l = v+2, \dots, L-1$, respectively, if and only if

$$E = \cos(\varphi), \quad (\text{H11})$$

independently of the actual choice of the parameters φ , $B \in \mathbb{C}$. Likewise, Eqs. (H3) and (H4) are seen to be fulfilled.

The parameter a_v [see below Eq. (H8)] can be fixed by choosing $l = v-1$ in Eq. (H1), implying

$$a_v = -a_{v-2} + 2Ea_{v-1} = -\alpha_{v-2} + 2E\alpha_{v-1} = \alpha_v, \quad (\text{H12})$$

where we exploited Eq. (H5) in the second step and Eqs. (H9) and (H11) in the last step. Analogously, one verifies by choosing $l = v+1$ in Eq. (H1) that $a_v = \beta_v$. Together with Eqs. (H5)–(H8), we thus obtain

$$a_l = \alpha_l = \sin(\varphi l), \quad \text{for } l \in \{1, \dots, v\}, \quad (\text{H13})$$

$$a_l = \beta_l = B \sin(\varphi(L+1-l)) \quad \text{for } l \in \{v, \dots, L\}. \quad (\text{H14})$$

Choosing $l = v$ in Eqs. (H13) and (H14) yields the first relation that the two remaining parameters φ and B have to fulfill, namely,

$$\sin(\varphi v) = B \sin(\varphi(L+1-v)) = B \sin(\varphi v), \quad (\text{H15})$$

where we exploited Eq. (115) in the last step. The second relation can be deduced from Eq. (H2) by rewriting it with Eqs. (H13) and (H14) in the form $\beta_{v+1} = -\alpha_{v-1} + (2E\alpha_m - p)\alpha_v$. Exploiting Eqs. (H9) and (H11), the right-hand side can be identified with $\alpha_{v+1} - p\alpha_v$. Observing Eqs. (H7) and (H8),

we thus obtain

$$B \sin(\varphi(L-v)) = \sin(\varphi(v+1)) - p \sin(\varphi v). \quad (\text{H16})$$

Our next goal is to show B must be nonzero by means of a proof by contradiction. Let us therefore assume that $B = 0$. With Eq. (H15), it follows that $\sin(\varphi v) = 0$ and then with (H16) that $\sin(\varphi(v+1)) = 0$. A straightforward calculation shows that

$$\sin(z) = 0 \quad \text{with } z \in \mathbb{C} \text{ implies } z = \pi n \quad \text{with } n \in \mathbb{Z}. \quad (\text{H17})$$

We thus can conclude that $\varphi(v+1) = \pi n$ and $\varphi n = \pi n'$ with $n, n' \in \mathbb{Z}$, implying $\varphi = \pi m$ with $m \in \mathbb{Z}$. With Eqs. (H13) and (H14), this yields $a_l = 0$ for all $l \in \{1, \dots, L\}$. According to the discussion below Eq. (39) this is not an admissible solution, thus completing our proof by contradiction.

In a next step, we take $B \neq 0$ for granted and separately discuss the cases $\sin(\varphi v) = 0$ and $\sin(\varphi v) \neq 0$. Considering first the case $\sin(\varphi v) = 0$, we can conclude from Eq. (H17) that $\varphi v = \pi n$ with $n \in \mathbb{Z}$. In particular, φ must be purely real. Similarly as before, $\varphi = 0$ would imply $a_l = 0$ for all l and can thus be excluded. Moreover, φ and $-\varphi$ lead to equivalent solutions in Eqs. (H11), (H13), and (H14) [see below Eq. (39)]. Likewise φ and $\varphi + 2\pi$ are equivalent. Hence, we can restrict ourselves to $\varphi \in (0, \pi)$. Altogether, the admissible φ values then must be of the form

$$\varphi = \frac{\pi k}{v} = \frac{2\pi k}{L+1} \quad \text{with } k \in \left\{1, \dots, v-1 = \frac{L-1}{2}\right\}, \quad (\text{H18})$$

where we exploited Eq. (116) in the last equalities. Finally, we can conclude from (H16) by rewriting $L-v$ as $L+1-(v+1)$ and observing Eq. (H18) and $\sin(\varphi v) = 0$ that

$$B \sin(-\varphi(v+1)) = \sin(\varphi(v+1)). \quad (\text{H19})$$

Similarly as below Eq. (H17), or directly from Eq. (H18) one finds that $\sin(\varphi(v+1)) \neq 0$, hence Eq. (H19) implies

$$B = -1. \quad (\text{H20})$$

Altogether, we thus obtained $(L-1)/2$ solutions of the form (H11), (H13), (H14), (H18), and (H20). A particularly important property of all those solutions is that they are of odd symmetry about $l = v$, meaning that $a_{v-j} = -a_{v+j}$ for all $j \in \{0, \dots, v-1\}$. Also quite remarkable is that the impurity strength p does not play any role. The reason is that $a_v = 0$ for all those solutions, hence the value of p in Eq. (H2) does not matter.

Next we turn the case $\sin(\varphi v) \neq 0$, implying with Eq. (H15) that

$$B = 1. \quad (\text{H21})$$

Together with Eq. (H16), this yields, after a short calculation, the following equation for φ :

$$2 \sin(\varphi) \cot(\varphi v) = p. \quad (\text{H22})$$

In a next step, one can show similarly as in Sec. IV A that with respect to the solutions of Eq. (H22) it is sufficient to focus on the following two cases. Case A: $\varphi \in (0, \pi)$. Case B: $\varphi = iy + n\pi$ with $y \in \mathbb{R}^+$ and $n \in \{0, 1\}$. In case A, one encounters, similarly as in Sec. IV B 1, a critical impurity

strength of the form (116), and one finds that whenever $|p| > p_c$ there are $v - 1$ solutions of Eq. (H22) of the form

$$\varphi = \frac{\pi(k + 1/2) + r_k}{v} \quad \text{with } k \in \left\{1, \dots, v - 1 = \frac{L - 1}{2}\right\}, \quad (\text{H23})$$

where the “remainders” r_k are bounded according to $|r_k| < \pi/2$ [cf. Eq. (65)]. Compared to Eq. (63), the main new feature of (116) is that p_c approaches zero for large L . Hence, the case $|p| < p_c$ is of minor interest and not further pursued here. Likewise, a more detailed discussion of r_k is quite similar to that in Sec. IV B 1 and therefore omitted.

Similarly as below Eq. (H20), the $(L - 1)/2$ solutions from Eqs. (H21) and (H23) are of even symmetry about $l = v$, meaning that $a_{v-j} = a_{v+j}$ for all $j \in \{0, \dots, v - 1\}$. Altogether, we thus obtained $L - 1$ solutions so far, half of them of odd and half of even symmetry. As in Sec. IV B 2, the still “missing” L th solution is obtained by exploring the above mentioned case B. Omitting the details, one arrives along these lines at

$$E = \pm \cosh(y), \quad (\text{H24})$$

$$a_l = (\pm 1)^l \sinh(y l) \quad \text{for } l \in \{1, \dots, v\}, \quad (\text{H25})$$

$$a_l = (\pm 1)^l \sinh(y(L + 1 - l)), \quad \text{for } l \in \{v, \dots, L\}, \quad (\text{H26})$$

where the plus sign applies when $p > p_c$ and the minus sign when $p < -p_c$. Moreover, y is defined as the (unique) solution of the equation

$$2 \sinh(y) \coth(yv) = |p| \quad (\text{H27})$$

with the property $y \in \mathbb{R}^+$. In particular, this solution (H25), (H26) is once again of even symmetry about $l = v$ [37].

Under the very weak extra assumption that $|p| \gg 1/L$ it follows with Eq. (115) that the solution of Eq. (H27) must satisfy $yv \gg 1$. Hence, the factor $\coth(yv)$ in Eq. (H27) can be approximated by unity, yielding

$$y = \text{arsinh}(|p|/2). \quad (\text{H28})$$

Under the even stronger assumption $1 \gg |p| \gg 1/L$, this yields the even simpler approximation

$$y = |p|/2. \quad (\text{H29})$$

On the other hand, for $p = p_c$ one readily verifies [similarly as in Eq. (91)] that

$$E = 1 \quad \text{and} \quad a_l = l = a_{L+1-l} \quad \text{for } l = 1, \dots, v \quad (\text{H30})$$

indeed satisfies Eqs. (H1)–(H4) even exactly, and analogously for $p = -p_c$ [37].

Finally, by employing the approximation (H29), one recovers Eq. (117) by means of analogous calculations as in Sec. IV D.

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- [1] C. Gogolin and J. Eisert, Equilibration, thermalization, and the emergence of statistical mechanics in closed quantum systems, *Rep. Prog. Phys.* **79**, 056001 (2016).
 - [2] T. Mori, T. N. Ikeda, E. Kaminishi, and M. Ueda, Thermalization and prethermalization in isolated quantum systems: A theoretical overview, *J. Phys. B* **51**, 112001 (2018).
 - [3] N. Shiraishi and H. Tasaki, Nature abhors a vacuum: A simple rigorous example of thermalization in an isolated macroscopic quantum system, *J. Stat. Phys.* **191**, 82 (2024).
 - [4] J. M. Deutsch, Quantum statistical mechanics in a closed system, *Phys. Rev. A* **43**, 2046 (1991).
 - [5] M. Srednicki, Chaos and quantum thermalization, *Phys. Rev. E* **50**, 888 (1994).
 - [6] M. Rigol, V. Dunjko, and M. Olshanii, Thermalization and its mechanism for generic isolated quantum systems, *Nature (London)* **452**, 854 (2008).
 - [7] L. D’Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics, *Adv. Phys.* **65**, 239 (2016).
 - [8] F. H. L. Essler and M. Fagotti, Quench dynamics and relaxation in isolated integrable quantum spin chains, *J. Stat. Mech.* (2016) 064002.
 - [9] E. Barouch, B. M. McCoy, and M. Dresden, Statistical mechanics of the XY model. I, *Phys. Rev. A* **2**, 1075 (1970); E. Barouch and B. M. McCoy, Statistical mechanics of the XY model. III, *Phys. Rev. A* **3**, 2137 (1971).
 - [10] G. Biroli, C. Kollath, and A. M. Läuchli, Effect of rare fluctuations on the thermalization of isolated quantum systems, *Phys. Rev. Lett.* **105**, 250401 (2010); V. Alba, Eigenstate thermalization hypothesis and integrability in quantum spin chains, *Phys. Rev. B* **91**, 155123 (2015); T. Mori, Weak eigenstate thermalization with large deviation bound [arXiv:1609.09776](https://arxiv.org/abs/1609.09776); E. Iyoda, K. Kaneko, and T. Sagawa, Fluctuation theorem for many-body pure quantum states, *Phys. Rev. Lett.* **119**, 100601 (2017); T. Kuwahara and K. Saito, Eigenstate thermalization from the clustering property of correlations, *Phys. Rev. Lett.* **124**, 200604 (2020).
 - [11] T. Farrelly, F. G. S. L. Brandão, and M. Cramer, Thermalization and return to equilibrium on finite quantum lattice systems, *Phys. Rev. Lett.* **118**, 140601 (2017).
 - [12] L. Dabelow, P. Vorndamme, and P. Reimann, Thermalization of locally perturbed many-body quantum systems, *Phys. Rev. B* **105**, 024310 (2022).
 - [13] P. Reimann and C. Eidecker-Dunkel, Thermalization in a simple spin-chain model, *Phys. Rev. B* **111**, 054312 (2025).
 - [14] M. Brenes, T. LeBlond, J. Goold, and M. Rigol, Eigenstate thermalization in a locally perturbed integrable system, *Phys. Rev. Lett.* **125**, 070605 (2020).
 - [15] M. Rigol, private communication regarding Ref. [14].
 - [16] L. F. Santos, Integrability of a disordered Heisenberg spin-1/2 chain, *J. Phys. A* **37**, 4723 (2004).
 - [17] O. S. Barisic, P. Prelovsek, A. Metavitsiadis, and X. Zotos, Incoherent transport induced by a single static impurity in a Heisenberg chain, *Phys. Rev. B* **80**, 125118 (2009).
 - [18] E. J. Torres-Herrera and L. F. Santos, Local quenches with global effects in interacting quantum systems, *Phys. Rev. E* **89**, 062110 (2014).
 - [19] M. Pandey, P. W. Claeys, D. K. Campbell, A. Polkovnikov, and D. Sels, Adiabatic deformations as a sensitive probe for quantum chaos, *Phys. Rev. X* **10**, 041017 (2020).

- [20] L. F. Santos, F. Pérez-Bernal, and E. J. Torres-Herrera, Speck of chaos, *Phys. Rev. Res.* **2**, 043034 (2020).
- [21] As usual, the units of the magnetic moments are chosen such that the spin-1/2 operators s_i^a can be expressed in the eigenbasis of s_i^z by the corresponding Pauli matrices σ_i^a as $s_i^a = \sigma_i^a/2$.
- [22] H. Touchette, Equivalence and nonequivalence of ensembles: thermodynamic, macrostate, and measure levels, *J. Stat. Phys.* **159**, 987 (2015).
- [23] F. G. S. L. Brandao and M. Cramer, Equivalence of statistical mechanical ensembles for non-critical quantum systems, [arXiv:1502.03263](https://arxiv.org/abs/1502.03263).
- [24] H. Tasaki, On the local equivalence between the canonical and the microcanonical ensembles for quantum spin systems, *J. Stat. Phys.* **172**, 905 (2018).
- [25] T. Kuwahara and K. Saito, Gaussian concentration bound and ensemble equivalence in generic quantum many-body systems including long-range interactions, *Ann. Phys.* **421**, 168278 (2020).
- [26] P. Reimann and C. Eidecker-Dunkel, Onsager's regression hypothesis adjusted to quantum systems, *Phys. Rev. B* **110**, 014306 (2024).
- [27] Our present notation is similar but not exactly identical to the one in Ref. [26]. In particular, our present Eq. (5) corresponds to Eq (11) in Ref. [26].
- [28] C. Eidecker-Dunkel and P. Reimann, Allosteric impurity effects in long spin chains, *Phys. Rev. B* **108**, 054407 (2023).
- [29] G. S. Uhrig, J. Hackmann, D. Stanek, J. Stolze, and F. B. Anders, Conservation laws protect dynamic spin correlations from decay: Limited role of integrability in the central spin model, *Phys. Rev. B* **90**, 060301(R) (2014).
- [30] A. M. Alhambra, J. Riddell, and L. P. Garcia-Pintos, Time evolution of correlation functions in quantum many-body systems, *Phys. Rev. Lett.* **124**, 110605 (2020).
- [31] H. Spohn, Interacting and noninteracting integrable systems, *J. Math. Phys.* **59**, 091402 (2018).
- [32] E. Lieb, T. Schultz, and D. Mattis, Two soluble models of an antiferromagnetic chain, *Ann. Phys.* **16**, 407 (1961).
- [33] H. B. Cruz and L. L. Goncalves, Time-dependent correlations of the one-dimensional isotropic XY model, *J. Phys. C: Solid State Phys.* **14**, 2785 (1981).
- [34] J. Stolze, V. S. Viswanath, and G. Müller, Dynamics of semi-infinite quantum spin chains at $T = \infty$, *Z. Phys. B* **89**, 45 (1992).
- [35] J. Stolze, A. Nöppert, and G. Müller, Gaussian, exponential, and power-law decay of time-dependent correlation functions in quantum spin chains, *Phys. Rev. B* **52**, 4319 (1995).
- [36] O. Derzhko, T. Krokhamalskii, and J. Stolze, Dynamics of the spin-1/2 isotropic XY chain in a transverse field, *J. Phys. A: Math. Gen.* **33**, 3063 (2000).
- [37] See also the general symmetry considerations around Eq. (41).
- [38] H. Tasaki, Heat flows from hot to cold: A simple rigorous example of thermalization in an isolated macroscopic quantum system, [arXiv:2404.04533](https://arxiv.org/abs/2404.04533).
- [39] C. Murthy and M. Srednicki, Relaxation to Gaussian and generalized Gibbs states in systems of particles with quadratic Hamiltonians, *Phys. Rev. E* **100**, 012146 (2019).
- [40] The latter finding is strictly speaking not yet sufficient to guarantee the occurrence of thermalization, see item (ii) at the end of Sec. IID.
- [41] Note that the mean-values of the long-time fluctuations are again quantitatively quite similar in Figs. 9 and 5, as can be deduced from the similarity of the red crosses in Figs. 3(b) and 6(b).
- [42] E. K. Sklyanin, Boundary conditions for integrable quantum systems, *J. Phys. A* **21**, 2375 (1988).
- [43] F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter, and G. R. W. Quispel, Surface exponents of the quantum XXZ, Ashkin-Teller and Potts models, *J. Phys. A* **20**, 6397 (1987).
- [44] N. Beisert, L. Fievet, M. de Leeuw, and F. Loebbert, Integrable deformations of the XXZ spin chain, *J. Stat. Mech.* (2013) P09028.
- [45] A. Hokkyo, Rigorous test for quantum integrability and nonintegrability, [arXiv:2501.18400](https://arxiv.org/abs/2501.18400).
- [46] G. Francica, T. J. G. Appolaro, N. Lo Gullo, and F. Plastina, Local quench, Majorana zero modes, and disturbance propagation in the Ising chain, *Phys. Rev. B* **94**, 245103 (2016).
- [47] More precisely speaking, for the end-impurities from Sec. IV, thermalization has been verified in Ref. [13] for all single-site observables of the form (11), while for the inner impurities from Sec. VI, only a subset of such single-site observables was covered. In both cases, the generalization from single-site to arbitrary local (multiple-site) observables readily follows by exploiting the “Gaussification”-results from Refs. [39].
- [48] N. Shiraishi and K. Matsumoto, Undecidability in quantum thermalization, *Nat. Commun.* **12**, 5084 (2021).
- [49] P. Sala, T. Rakovszky, R. Verresen, M. Knap, and F. Pollmann, Ergodicity breaking arising from Hilbert space fragmentation in dipole-conserving Hamiltonians, *Phys. Rev. X* **10**, 011047 (2020); T. Rakovszky, P. Sala, R. Verresen, M. Knap, and F. Pollmann, Statistical localization: From strong fragmentation to strong edge modes, *Phys. Rev. B* **101**, 125126 (2020); S. Moudgalya, B. A. Bernevig, and N. Regnault, Quantum many-body scars and Hilbert space fragmentation: A review of exact results, *Rep. Prog. Phys.* **85**, 086501 (2022).
- [50] P. Reimann and C. Eidecker-Dunkel, Absence of thermalization after a local quench and strong ETH violation, figshare, Dataset (2025), <https://doi.org/10.6084/m9.figshare.29900183.v1>.
- [51] M. Kliesch, C. Gogolin, M. J. Kastoryano, A. Riera, and J. Eisert, Locality of temperature, *Phys. Rev. X* **4**, 031019 (2014); H. Araki, Gibbs states of a one dimensional quantum lattice, *Commun. Math. Phys.* **14**, 120 (1969); Y. M. Park, The cluster expansion for classical and quantum lattice systems, *J. Stat. Phys.* **27**, 553 (1982); Y. M. Park and H. J. Yoo, Uniqueness and clustering properties of Gibbs states for classical and quantum unbounded spin systems, **80**, 223 (1995).