Matrix Product Symmetries and Breakdown of Thermalization from Hard Rod Deformations

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We construct families of exotic spin-1/2 chains using a procedure called "hard rod deformation." We treat both integrable and nonintegrable examples. The models possess a large noncommutative symmetry algebra, which is generated by matrix product operators with a fixed small bond dimension. The symmetries lead to Hilbert space fragmentation and to the breakdown of thermalization. As an effect, the models support persistent oscillations in nonequilibrium situations. Similar symmetries have been reported earlier in integrable models, but here we show that they also occur in nonintegrable cases.

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Introduction.—Ergodicity is a central concept in mathematics and physics, and it underlies statistical physics and thermodynamics. Today it is understood that in isolated quantum many body systems thermalization is guaranteed by the eigenstate thermalization hypothesis [1], which in principle states that in generic systems most pure states are indistinguishable from thermal ensembles.

In the last two decades, considerable interest has been devoted to the following questions: What types of ergodicity breaking can exist in quantum many body systems? and what are the underlying physical mechanisms? A common property appears to be the presence of exotic symmetries, which lead to unconventional conservation laws, thus preventing thermalization.

Famous examples are the integrable models, which possess an infinite set of conservation laws [2,3]. Such models equilibrate to states described by the generalized Gibbs ensemble [4,5] and they support ballistic transport [6,7]. Many body localization provides another mechanism, where strong disorder leads to the emergence of an extensive set of local integrals of motion [8].

Unconventional symmetries are seen also in models with Hilbert space fragmentation [9–14]. In these models there is an exponentially growing number of kinetically disconnected sectors in the Hilbert space. Families of such models have a symmetry algebra whose dimension also grows exponentially with the volume [15]. These extra symmetries lead to the breakdown of ergodicity and to the slowdown of transport (for classical counterparts of this phenomenon see Refs. [16,17]). Fragmented models are typically nonintegrable, but integrable examples are also known [15,18,19].

In this Letter, we uncover a new mechanism for Hilbert space fragmentation. Using a procedure called "hard rod deformation" we construct strongly interacting spin-1/2 chains with hidden exotic symmetries, given by matrix product operators (MPOs) with small bond dimension. Our models are generally nonintegrable, and the algebra of the MPO symmetries is not commutative. The MPO symmetries ensure exact degeneracies among states in different fragmented sectors. This leads to exotic dynamical effects, such as nondecaying oscillations in nonequilibrium situations.

Previously such phenomena were observed only for integrable models [15,18,20,21], where the extra symmetries are given typically by MPOs [3]. Our work is unique: it shows that (noncommutative) MPO symmetries can be found even in nonintegrable spin chains. This provides a new way of ergodicity breaking, and it also enriches our understanding of symmetries and their implications in quantum spin chains.

Models.—Our main models are spin-1/2 chains. The local basis states are denoted as $|\uparrow\rangle$, $|\downarrow\rangle$, and we use the short notations X_j, Y_j, Z_j for the Pauli matrices acting on site j. We use the local projectors $P_j = (1 + Z_j)/2$ and $N_j = (1 - Z_j)/2$, and also the two-site projectors $\Pi^{\pm}_{j,k} = (1 \pm Z_j Z_k)/2$. In all cases we treat extensive and translationally invariant Hamiltonians defined as $H = \sum_{j=1}^{L} h(j)$, with an operator density $h(j)$ which is a short range operator. We work with periodic boundary conditions.

We treat a family of models defined by

$$h(j) = h_f(j) + \Delta h_{ZZ}(j) + \kappa h_{ni}(j). \tag{1}$$

The first term is the kinetic part of the Hamiltonian, describing controlled hopping:

$$h_f(j) = (X_{j+1}X_{j+2} + Y_{j+1}Y_{j+2})\Pi^{+}_{j,j+3}. \tag{2}$$

The other two terms describe interactions, they are diagonal in the given basis, and they span four and six sites, respectively:

$$h_{ZZ}(j) = \Pi^+_{j,j+3}\Pi^-_{j+1,j+2},$$
$$h_{ni}(j) = \Pi^+_{j,j+5}\Pi^-_{j+1,j+2}\Pi^-_{j+2,j+3}\Pi^-_{j+3,j+4}. \qquad (3)$$

Without interactions ($\Delta = \kappa = 0$) we have the folded XXZ model, which describes the high temperature dynamics of the XXZ Heisenberg spin chain in the large anisotropy limit [18,20,22–24]. The folded XXZ model also appeared in [25], and it is closely related to stochastic models treated in [26]. It is an integrable model, which can be solved exactly by the Bethe ansatz [18,20].

Switching on $\Delta \neq 0$ but keeping $\kappa = 0$ we obtain the so-called hard rod deformed XXZ model introduced in [19]. It is also an integrable model, which is closely related to the actual XXZ model and also to the constrained models of [27–29]. Switching on $\kappa \neq 0$ breaks integrability [30].

Dynamics.—The kinetic term in (2) generates the transitions $|\uparrow\uparrow\downarrow\uparrow\rangle \leftrightarrow |\uparrow\downarrow\uparrow\uparrow\rangle$ and $|\downarrow\uparrow\downarrow\downarrow\rangle \leftrightarrow |\downarrow\downarrow\uparrow\downarrow\rangle$ on four sites. As an effect, single down and up spins can propagate freely in a background of up and down spins, respectively. On the other hand, states with isolated domain walls are frozen. For example, the kinetic term acts as zero on the local configuration $|\uparrow\uparrow\downarrow\downarrow\rangle$. It follows, that any state which consists only of domains (sequences of spins with the same orientation, being longer than two) are frozen. However, nontrivial dynamics arises when a single particle scatters on an isolated domain wall. In such a case, we observe particle-hole transmutation: when an incoming particle (for example a down spin in a background of up spins) meets a domain wall, it continues its path as a hole (in this case, as an up spin in a background of down spins). As a by-product, the domain wall gets displaced by two sites. This dynamical phenomenon was treated in detail in [18,36,37].

It follows from the structure of the kinetic term and the interaction terms, that the following two $U(1)$ charges are conserved for arbitrary Δ and κ:

$$Q_1 = \sum_j Z_j, \qquad Q_2 = \sum_j Z_j Z_{j+1}. \qquad (4)$$

Here Q_1 is the global magnetization, while Q_2 is (up to normalization) the "domain wall number."

Matrix product symmetries.—Below we show that our model possesses exotic symmetries for generic values of the coupling constants, also in the nonintegrable case. These symmetries are represented by MPOs, which commute with the Hamiltonian. An MPO is a one-dimensional tensor network where each tensor has two external indices (corresponding to the physical spaces) and two internal indices (corresponding to an auxiliary space $V_a = \mathbb{C}^D$ with an appropriate constant $D \geq 2$).

We introduce the elementary tensor as a linear operator $\mathcal{L}_{a,j}$ which acts on the tensor product space $V_a \otimes V_j$, where $V_j = \mathbb{C}^2$ is the physical space at site j. The MPO with periodic boundary conditions is then defined as

$$\mathcal{T} = \mathrm{Tr}_a[\mathcal{L}_{a,L}\ldots\mathcal{L}_{a,2}\mathcal{L}_{a,1}]. \qquad (5)$$

We say that $\mathcal{T}$ is an MPO symmetry if it commutes with the Hamiltonian in every volume L.

A distinguishing property of an MPO is that its operator space entanglement entropy [38,39] is bounded from above by $2\log(D)$. Therefore it satisfies the "area law" of entanglement [40]. In the special case of $\mathcal{L}_{j,a} = o_j$ with o being a one-site operator the MPO becomes proportional to a product operator. Therefore, an MPO symmetry can be seen as a generalization of strictly local internal symmetries.

MPO symmetries are known to exist in integrable spin chains with local interactions [3,41]. In those models the tensor $\mathcal{L}$ is called the Lax operator, and it depends on a complex variable (spectral parameter) and possibly some discrete variables too. The resulting MPOs are called transfer matrices, and they form a commuting family. Extensive conserved charges with short range operator densities are derived from such families of MPOs.

In our family of models commuting transfer matrices have been found in the integrable cases in [18,19]. They fit into the canonical framework of Yang-Baxter integrable spin chains [41], generalized to spin chains with medium range interaction [42]. However, those symmetries get broken after switching on $\kappa \neq 0$.

In contrast, we derive new MPO symmetries that hold in both the integrable and nonintegrable cases. In order to derive these symmetries first we perform a sequence of transformations on our models.

Bond model.—Following [18,20] we perform a so-called bond-site transformation, which we define on the level of the basis states in the computational basis. The idea is to put variables on the bonds between the sites, such that the values ± 1 on the bond represent whether the two neighboring spins have the same or different values. The original Hamiltonian is invariant with respect to global spin reflection, therefore it will generate local dynamics for the bond variables. Basis states in the bond model will be denoted as $|\circ\rangle$ (empty site or spin up) and $|\bullet\rangle$ (occupied site or spin down), which correspond to identical and opposite spins on neighboring sites of the original model, respectively. For more details about the transformation see Ref. [30].

In the bond model the nonzero kinetic transitions are $|\circ\bullet\bullet\rangle \leftrightarrow |\bullet\bullet\circ\rangle$. These are interpreted as a one site translation of dimers or "hard rods," which are particles spanning two sites. They are the mobile particles in these models, and they motivated the use of the expression "hard rod deformation" [19]. In contrast, single $|\bullet\rangle$ states embedded in a vacuum of empty sites are immobile on their own. They are displaced when a mobile particle scatters on them.

The XXC models.—The bond models can be mapped further to spin chains with three-dimensional local spaces. This mapping is nonlocal and volume changing, and it appeared among others in [18] but also much earlier in [26] (see also [43]). The mapping is defined as follows.

In the computational basis the states can be seen as a sequence of ∘ and • "characters," and these sequences are translated into sequences consisting of the numbers 0, 1, and 2. The original sequence is "read" from the left to the right. If a ∘ is encountered then one writes down a 1. If a • is encountered, then one also reads the next character. In case of a • or ∘ one writes down a 0 or a 2, respectively. This gives the local transformation rules

$$|\circ\rangle \to |1\rangle, \qquad |\bullet\bullet\rangle \to |0\rangle, \qquad |\bullet\circ\rangle \to |2\rangle. \tag{6}$$

This mapping is volume changing: the length of the new sequence depends on the content of the original sequence. This implies that different sectors of the Hilbert space of the original model will be mapped to Hilbert spaces of the new spin chain with varying lengths.

The transformation induces a mapping for the Hamiltonians. The transformation of the basis states is strongly nonlocal, therefore locality is typically lost on the level of the Hamiltonians. Nevertheless it is possible to select certain local Hamiltonians which remain local after the mapping [18,19,26,43], and our family of models also has this property.

We introduce notations for operators acting on the three-dimensional local spaces. We have $s_\alpha^- = |\alpha\rangle\langle 0|$ with $\alpha = 1$, 2 and they can be arranged into a two-dimensional vector $\mathbf{s}^- = (s_1^-, s_2^-)$. Furthermore $\mathbf{s}^+ = (\mathbf{s}^-)^\dagger$, and we also introduce the projectors $n = |0\rangle\langle 0|$, $p = |1\rangle\langle 1| + |2\rangle\langle 2|$. Direct computation shows [30] that our model Hamiltonians are eventually mapped to short range Hamiltonians with density

$$h^C(j) = h_f^C(j) + \Delta h_{ZZ}^C(j) + \kappa h_{ni}^C(j), \tag{7}$$

with

$$\begin{aligned} h_f^C(j) &= \mathbf{s}^-{}_j \cdot \mathbf{s}^+{}_{j+1} + \mathbf{s}^+{}_j \cdot \mathbf{s}^-{}_{j+1}, \\ h_{ZZ}^C(j) &= n_j p_{j+1} + p_j n_{j+1}, \\ h_{ni}^C(j) &= n_j n_{j+1} p_{j+2} + p_j n_{j+1} n_{j+2}. \end{aligned} \tag{8}$$

The model with $\Delta = \kappa = 0$ appeared in [44] and it is closely related to the strong coupling limit of the Hubbard model (also known as the $t-0$ model). The model with $\Delta \neq 0$ but $\kappa = 0$ appeared in [45] (and in a special case in [26]) and it was called the XXC model. The nonintegrable perturbation appears to be new; we call it the deformed XXC model.

Spin-charge separation.—The kinetic terms in (7) generate the transitions $|01\rangle \leftrightarrow |10\rangle, |02\rangle \leftrightarrow |20\rangle$. The transition $|12\rangle \leftrightarrow |21\rangle$ is forbidden, thus the relative ordering of the basis states $|1\rangle$ is $|2\rangle$ cannot be changed during time evolution.

We can regard the local state $|0\rangle$ as the vacuum, and the states $|1\rangle$ and $|2\rangle$ as a particle (charge) with an internal degree of freedom (spin). Then we can perform a spin-charge separation: we specify each basis state by giving the positions and the spins of the particles. The Hamiltonians are such that the spin-charge separation leads to exactly decoupled dynamics, the spin part of the wave function is a constant of motion, and it does not influence the motion of the particles. This is a nontrivial property, which we prove in detail in [30].

This phenomenon was already observed in a number of works dealing with similar models [18,26,43,46,47]. It induces Hilbert space fragmentation: different values of the spin pattern all correspond to different irreducible sectors in the Hilbert space. This phenomenon underlies the existence of the exotic symmetries of all our models. Furthermore, it allows for exact solutions of real time dynamics in similar models [46–50].

Symmetries for XXC.—We construct MPO symmetries for the deformed XXC models, and afterwards we generalize the construction for our original family (1).

In the deformed XXC models we construct MPOs with fixed bond dimension two. The key idea is that the MPOs should act only on the spin degrees of freedom, while leaving the particle positions intact [26]. This will guarantee that the MPOs commute with the Hamiltonian. Generally such operators are very nonlocal, but there exist representatives with the desired MPO structure. The majority of our results for the MPOs are new.

In the XXC case we expand $\mathcal{L} = I \otimes |0\rangle\langle 0| + \sum_{\alpha,\beta=1,2} F^{(\alpha,\beta)} \otimes |\alpha\rangle\langle\beta|$. Here I and $F^{(\alpha,\beta)}$ are five matrices of size 2×2 which act on the auxiliary space, and specifically I is the identity matrix. Such an MPO acts as the identity on every local vacuum state $|0\rangle$, but typically it has a nontrivial action on the spin degrees of freedom. The resulting MPOs do not change the position of the particles, but they can modify the spin pattern.

We consider two subclasses of such MPOs. In one class the resulting MPOs are diagonal, which can be achieved by setting $F_{12} = F_{21} = 0$. Such MPOs do not change the spin pattern, but their eigenvalues (diagonal matrix elements) do depend on it. These MPOs all commute with each other and also the Hamiltonian.

The number of independent parameters of these MPOs can be reduced to five, and representatives can be chosen for example as

$$F^{(1,1)} = \begin{pmatrix} x & y \\ y & z \end{pmatrix}, \qquad F^{(2,2)} = \begin{pmatrix} u & 0 \\ 0 & v \end{pmatrix}. \tag{9}$$

The second class of MPO symmetries changes the spin pattern. We concentrate on those MPOs which conserve the number of $|1\rangle$ and $|2\rangle$ states. This can be achieved by the following matrices with five independent parameters:

$$F^{(1,2)} = (F^{(2,1)})^\dagger = \gamma\sigma^-,$$
$$F^{(1,1)} = \begin{pmatrix} \alpha & \\ & \delta \end{pmatrix}, \qquad F^{(2,2)} = \begin{pmatrix} \beta & \\ & \varepsilon \end{pmatrix}. \tag{10}$$

Our diagonal MPOs are included in the results of [15], but the off-diagonal ones appear to be new.

Main results.—Now we pull back these MPO symmetries to the original family of models given by (1). This is a nontrivial task, because the transformation rule (6) causes strong nonlocality. However, the action of the two classes of MPOs that we introduced can be emulated by an MPO with fixed bond dimension even in the original model. The auxiliary dimension needs to be enlarged in order to deal with the nonlocal effects, but afterwards it will not depend on the volume. It is important that the transformation between the models cannot be described by an MPO with fixed bond dimension: This happens only for the selected symmetry operators that we construct.

In order to find the actual MPOs, we use the techniques discussed in [51]. We view the MPO as an "automaton" with a finite number of internal states, which are changed as the MPO acts on the physical spin chain. These internal states and their transitions will encode the rules (6) and also the bond-site transformation.

We construct two families of MPO symmetries which we denote as $\mathcal{T}^d$ and $\mathcal{T}^o$, corresponding to the diagonal and off-diagonal classes above. In both cases we expand $\mathcal{L} = \mathcal{A}\otimes|\uparrow\rangle\langle\uparrow| + \mathcal{B}\otimes|\uparrow\rangle\langle\downarrow| + \mathcal{C}\otimes|\downarrow\rangle\langle\uparrow| + \mathcal{D}\otimes|\downarrow\rangle\langle\downarrow|$, where $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\mathcal{D}$ are sparse matrices of size $D\times D$ acting on the auxiliary space.

For the family $\mathcal{T}^d$ the auxiliary space has dimension $D = 8$ and we view it as the tensor product $\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2$. The MPOs depend on five independent parameters, and they are diagonal, which is ensured by $\mathcal{B} = \mathcal{C} = 0$. They commute with each other and also with the local charges Q_1 and Q_2. The concrete matrices are

$$\begin{aligned}
\mathcal{A} &= N\otimes F^{(1,1)}\otimes P + \sigma^+\otimes F^{(2,2)}\otimes\sigma^- \\
&\quad + N\otimes I\otimes\sigma^- + P\otimes I\otimes\sigma^+, \\
\mathcal{D} &= P\otimes F^{(1,1)}\otimes P + \sigma^-\otimes F^{(2,2)}\otimes\sigma^- \\
&\quad + P\otimes I\otimes\sigma^- + N\otimes I\otimes\sigma^+,
\end{aligned} \tag{11}$$

where N and P are projectors introduced above, and $F^{(1,1)}$ and $F^{(2,2)}$ are given in (9).

In the case of the family $\mathcal{T}^o$ the auxiliary space has dimension $D = 10$, and $\mathcal{L}$ depends on five independent parameters. These MPOs are generally not diagonal, and they do not commute with each other. Concrete matrix elements are [30]

$$\begin{aligned}
&\mathcal{A}_{1,2} = \mathcal{A}_{3,4} = \mathcal{A}_{5,4} = \mathcal{A}_{7,6} = \mathcal{A}_{9,10} = 1, \\
&\mathcal{D}_{2,1} = \mathcal{D}_{4,5} = \mathcal{D}_{6,7} = \mathcal{D}_{8,9} = \mathcal{D}_{10,9} = 1, \\
&\mathcal{A}_{6,6} = \mathcal{D}_{1,1} = \alpha, \qquad \mathcal{A}_{2,6} = \mathcal{D}_{7,1} = \beta, \\
&\mathcal{A}_{4,6} = \mathcal{B}_{1,3} = \mathcal{C}_{6,8} = \mathcal{D}_{9,1} = \gamma, \\
&\mathcal{B}_{3,3} = \mathcal{B}_{5,3} = \mathcal{C}_{8,8} = \mathcal{C}_{10,8} = \delta, \\
&\mathcal{B}_{9,3} = \mathcal{C}_{4,8} = \varepsilon.
\end{aligned} \tag{12}$$

These MPOs commute with Q_2, because they originate from the MPOs given by (10), which conserve the "spin" in the XXC models, eventually leading to conservation of the number of domain walls in the original models. However, they break the global magnetization Q_1, because they generate a displacement of the domain walls.

The MPOs do not depend on the parameters Δ, κ: they are symmetries for the full family of models. The diagonal MPOs commute with the Hamiltonian densities $h(j)$ separately: they belong to the commutant algebra [15]. The off-diagonal ones commute only with the full Hamiltonian.

Persistent oscillations.—We explore the dynamical consequences of the MPO symmetries. We consider real time evolution started from a selected initial state $|\Psi_0\rangle = \otimes_{j=1}^{L}(|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$, which is a state completely polarized in the x direction. This state breaks the $U(1)$ invariance associated with the global magnetization. We consider time evolution generated by $H + hQ_1$, where H is given by (1) with generic values of the coupling constants and h is a magnetic field. We focus on the time evolution of the local observable X_j; for simplicity we will drop the site index j in the notation.

We performed the numerical computation of the real time evolution using the iTEBD method [52,53]. Our data are presented in Fig. 1, for details see Ref. [30].

The local operator X breaks the $U(1)$ symmetry generated by Q_1. In the absence of extra symmetries it is expected that the mean value $\langle\Psi_0|X(t)|\Psi_0\rangle$ drops to zero in the long time limit, for both integrable and nonintegrable cases. However, in our case we observe that $X(t)$ has a nonzero stationary value for $h = 0$, and for $h \neq 0$ it shows

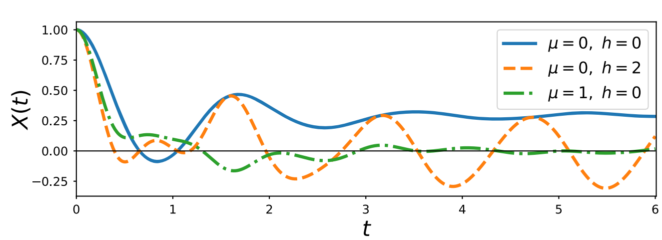

FIG. 1. Real time dynamics from a selected initial state, with a nonintegrable Hamiltonian with $\Delta = 0.2$ and $\kappa = 0.5$. The second curve is obtained after adding a magnetic field h. The third curve is obtained after adding a perturbing term H' which breaks the MPO symmetries.

nondecaying oscillations with frequency $2h$ [54]. The reason for this phenomenon is that the off-diagonal MPO symmetries also break the given $U(1)$ charge. Adding one more perturbation $H' = \mu \sum_j Z_j Z_{j+1} Z_{j+2}$ breaks all MPO symmetries, and in this case we observe relaxation to zero, as expected.

Persistent oscillations were reported earlier in relation with integrability [18,21] and also in models with quantum scars [11,12,55]. The novelty of the present results is that we find the same effects in nonintegrable models, explained by the MPO symmetries. In our models ergodicity breaking extends over essentially the full Hilbert space, therefore the phenomenon is not related to quantum scars. In fact, the same effects would be observed for almost all product states of the form $|\Psi_0\rangle = \otimes_{j=1}^{n} |\psi_l\rangle$, where $|\psi_l\rangle$ is an l-site state breaking $U(1)$ invariance, and $L = nl$. The reason is that almost all such states overlap with exponentially many fragmented sectors from the Hilbert space.

Discussion.—Our mechanism for Hilbert space fragmentation allows for unusual MPO symmetries, which hold in the integrable and nonintegrable cases too. The MPO symmetries generate a noncommutative algebra, therefore the models should be seen as having quantum fragmentation. In the literature there have been few examples for quantum fragmentation [14,15,56], and our models provide a new mechanism for this. Also, they appear to be the first examples of nonintegrable models with off-diagonal MPO symmetries.

Our models have strong fragmentation [9], because the symmetries affect the whole spectrum in a nontrivial manner. This leads to exponentially large degeneracies for almost all states, but the concrete degeneracies depend on the state [18,19]. Our symmetry operators are similar in essence to the "statistically localized integrals of motion" found in [57], but it is a novel result that we construct them in the form of MPOs with low bond dimension.

The XXC models that appeared in our study have the special property that spin-charge separation is exact, the spin pattern is always conserved, and it does not influence the charge degrees of motion. It was argued in [47] that in such models the spin transport has anomalous fluctuations. This is believed to be true also for the folded XXZ model [37,47], although the rigorous proofs of [47] do not apply in that case. We conjecture that our family of models also displays anomalous fluctuations, in both the integrable and nonintegrable cases.

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