Universal spin dynamics in infinite-temperature one-dimensional quantum magnets

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Universal Spin Dynamics in Infinite-Temperature One-Dimensional Quantum Magnets

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We address the nature of spin dynamics in various integrable and non-integrable, isotropic and anisotropic quantum spin-S chains, beyond the paradigmatic $S = 1/2$ Heisenberg model. In particular, we investigate the algebraic long-time decay $\propto t^{-1/z}$ of the spin-spin correlation function at infinite temperature, using state-of-the-art simulations based on tensor network methods. We identify three universal regimes for the spin transport, independent of the exact microscopic model: (i) superdiffusive with $z = 3/2$, as in the Kardar-Parisi-Zhang universality class, when the model is integrable with extra symmetries such as spin isotropy that drive the Drude weight to zero, (ii) ballistic with $z = 1$ when the model is integrable with a finite Drude weight, and (iii) diffusive with $z = 2$ with easy-axis anisotropy or without integrability, at variance with previous observations.

Introduction.— Understanding equilibrium and out-of-equilibrium dynamics of interacting quantum systems remains one of the most strenuous problems in modern physics. From a phenomenological perspective, taking into account the few conservation laws of a system such as energy, momentum and particle number, one can derive classical hydrodynamic equations to describe a coarse-grained thermodynamic version of the microscopic model [1, 2]. Yet, some systems possess an extensive set of conservation laws, strongly constraining their dynamics and endowing them with exotic thermalization and transport properties [3–8]. They are known as *integrable* systems and are ubiquitous in the low-dimensional quantum world, with experimentally relevant examples from magnets to Bose gases [9–14].

Two simple paradigms of how a conserved quantity spreads are exemplified by ordinary thermalizing systems with diffusion on the one hand, and free-particle systems (a simple kind of integrable system) with ballistic transport on the other. After many years and much analytical and numerical progress [3, 6, 15–24], the existence of both regimes in the spin-half XXZ model, which is a version of the Heisenberg model with uniaxial anisotropy in the interaction, has been understood in detail, with quantitative explanations of the Drude weight that governs the amount of ballistic transport. Numerical studies on this model provide a stringent test of the generalized hydrodynamical approach to time evolution of densities in ballistic regimes of integrable models [19, 20, 25].

Unexpectedly, a numerical study observed a third behavior at the isotropic (Heisenberg) point of this model [26, 27]: spin dynamics at infinite temperature were characterized by superdiffusion with the same dynamical critical exponent $z = 3/2$, defined below, that appears in the *classical*, *stochastic* Kardar-Parisi-Zhang (KPZ) universality class [28]. This led to additional studies that explained how the diffusion constant must become infinite at the Heisenberg point [29] and showed agreement with the full KPZ scaling function [27, 30–33]. Note that this emergence of superdiffusion and KPZ universality from quantum models is different from the superdiffusion with $z = 1$ that emerges in systems with momentum conservation [34, 35] or the variable dynamical critical exponent at low temperatures in Luttinger liquids [36]. It also does not seem to follow from the useful mapping between a classical exclusion process in the KPZ universality class and *statics* of the spin-half XXZ model, for a review, see e.g., Ref. 37.

The main point of this paper is to study infinite-temperature dynamics in a variety of one-dimensional quantum magnets with $S > 1/2$, with and without integrability and isotropy, in order to isolate the requirements for KPZ superdiffusion. We find several new examples of higher-spin chains that all have dynamical critical exponent $z = 3/2$, despite having variable symmetries and interactions. These can be viewed as interpolating between the $S = 1/2$ results and recent studies of a classical integrable spin chain [38]. We find that the occurrence of superdiffusion with $S = 1$ is not limited to the isotropic case, but that it does require integrability; more precisely, we find that superdiffusion is not present in the simplest nearest-neighbor models with $S = 1$, $3/2$ and 2, contrary to recent proposals [39], and we explain what we believe to be missing in that theoretical analysis.

Investigating spin dynamics.— To investigate the spin dynamics in quantum spin-S systems, we focus on the infinite-temperature local spin-spin correlation function,

$$\mathcal{C}(L,t) = \frac{3}{S(S+1)}\left\langle S^z_{L/2}(t)\, S^z_{L/2}(0)\right\rangle, \tag{1}$$

where $S^z_{L/2}$ is the spin operator component along the quantization axis at position $L/2$ in a system of total length L, $\langle\cdot\rangle \equiv \mathrm{tr}(\cdot)/(2S+1)^L$ denotes the infinite temperature thermal average and $S^z_r(t) = \mathrm{e}^{i\mathcal{H}t} S^z_r \mathrm{e}^{-i\mathcal{H}t}$ is the time-dependent operator in the Heisenberg picture, with $\mathcal{H}$ the Hamiltonian describing the system. The prefactor $3/S(S+1)$ in Eq. (1) ensures that $\mathcal{C}(L, t = 0) = 1$.

We consider a wide range of integrable and non-integrable, isotropic and anisotropic quantum spin-S chains described by Hamiltonians of the form $\mathcal{H} = \sum_j \hat{h}_{j,j+1}$ with $\hat{h}_{j,j+1}$ the local Hamiltonian density. All models conserve the total magnetization $S^z_{\mathrm{tot}} = \sum_j S^z_j$,

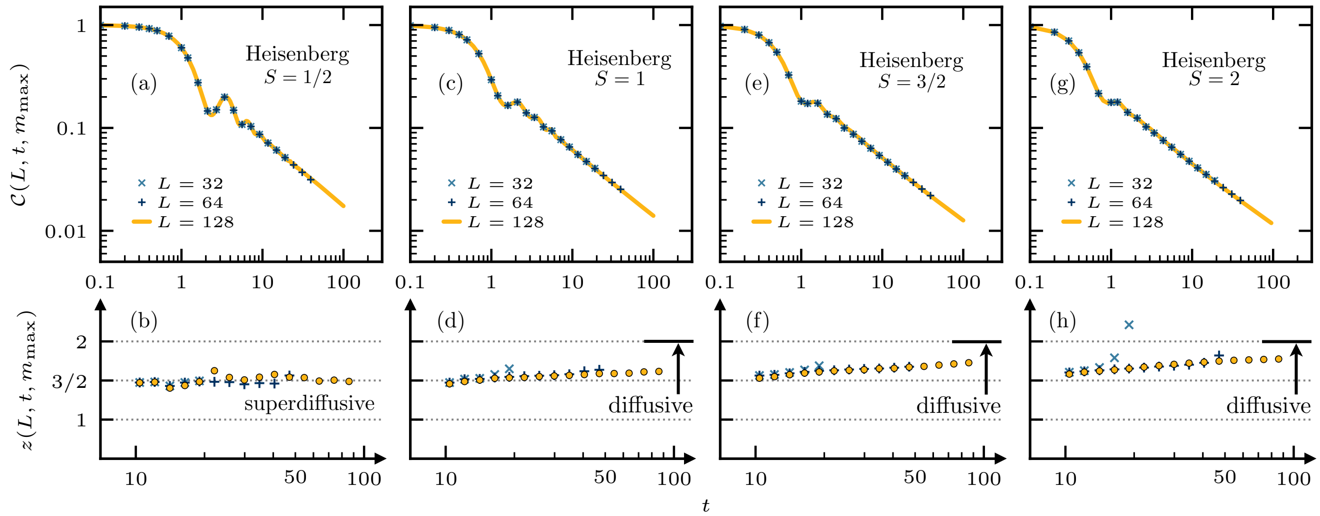

FIG. 1. Top panels (a, c, e, g): Infinite temperature spin-spin correlation function (1) for the isotropic one-dimensional Heisenberg model (3) for spin values $S = 1/2$, 1, 3/2 and 2. Bottom panels (b, d, f, h): Extracted dynamical exponent $z(L, t, m_{\max})$ by performing curve-fitting inside a sliding window of data points in order to reliably the infinite-length and infinite-time value of the power-law decay as in Eq. (2). Only the spin-1/2 case is integrable and show consistent superdiffusive dynamical behavior over time with $z(L, t, m_{\max}) = 3/2$. For the larger spin-S models, the dynamical exponent value systematically increases when varying the curve-fitting window toward longer times with $z \to 2$, supporting diffusive dynamics. Additional analyses are available in the supplemental material.

and some additionally conserve the total spin $\boldsymbol{S}_{\text{tot}} = \sum_j \boldsymbol{S}_j$, where $\boldsymbol{S}_j = \left(S_j^x, S_j^y, S_j^z\right)$ is the usual spin-S operator at site j, making them fully isotropic. Because of S_{tot}^z conservation, in the hydrodynamic limit, the spin fluctuations captured by the spin-spin correlation function (1) are expected to decay with a power-law tail at late time for infinitely large systems,

$$\lim_{t\to\infty} \lim_{L\to\infty} \mathcal{C}(L, t) \sim t^{-1/z}, \tag{2}$$

with z the dynamical exponent characterizing the nature of the spin dynamics and spin transport in the system: $z = 2$ for diffusion, $z = 3/2$ for KPZ-type anomalous diffusion or superdiffusion, and $z = 1$ for ballistic dynamics.

We compute the spin-spin correlation function (1) numerically using matrix product states (MPS) calculations [40] together with the purification method [41]. The time evolution is performed through the time-evolving block decimation algorithm [42] along with a fourth order Trotter decomposition [43] of time step $\delta_t = 0.1$. The control parameter of the numerical simulations is the bond dimension m of the MPS whose convergence is thoroughly studied in the supplemental material. In the following, we only show data for the largest bond dimension computationally available $m \equiv m_{\max}$. In practice one only has access to finite systems L and is limited in the maximum time t. Therefore, it is instructive to perform curve-fitting inside a sliding window of data points in order to reliably extract the infinite-length and infinite-time value of the dynamical exponent z [44].

The Heisenberg model.—We first consider the paradigmatic SU(2)-symmetric Heisenberg model,

$$\hat{h}_{j,j+1} = \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}, \tag{3}$$

for $S = 1/2$, 1, 3/2 and 2, and which is integrable exclusively in the spin-1/2 case [45, 46]. The correlation function (1) and the extracted dynamical exponent z are shown in Fig. 1. Superdiffusive behavior with $z = 3/2$ is unambiguously observed for the $S = 1/2$ case, in agreement with previous results [26, 27, 29, 30, 47, 48]. $z = 3/2$ is the same dynamical scaling exponent as of the KPZ universality class [28], and the relation has been confirmed by showing that the infinite temperature spin-spin correlation function obeys KPZ scaling [27, 30]. For larger spins $S \geq 1$, the dynamical exponent value systematically increases when varying the curve-fitting window toward longer times with $z \to 2$, supporting diffusive dynamics.

Our result of diffusive dynamics in these non-integrable cases is perhaps not too surprising, but there is a relatively long crossover before reaching this limit, and the fact that at short time $z \approx 3/2$ can be misleading. For instance, based on calculations on a low-energy effective quantum field theory for the Heisenberg model (3), namely the non-linear sigma model [49–51], the authors of Ref. 39 claim that anomalous spin transport is present in any spin-S Heisenberg chain at low temperature, and persists at high temperature as corroborated by simulations on the exact spin-1 microscopic model. However their simulations do not go to long enough time to observe the increase of z as we do. The superdiffusive dynamics that they obtain is an artifact of the low-energy

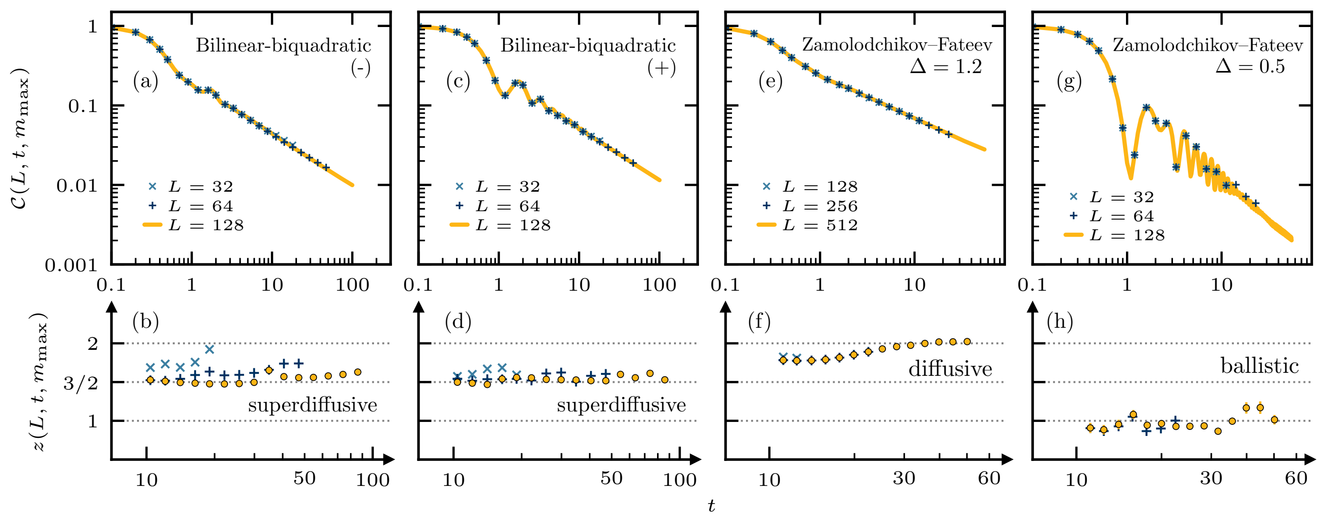

FIG. 2. Top panels (a, c, e, g): Infinite temperature spin-spin correlation function (1) for various one-dimensional spin-1 models. First, the isotropic bilinear-biquadratic Heisenberg chain defined in Eq. (4) for two different signs of the biquadratic term (panels a and c respectively). Then, the Zamolodchikov-Fateev model (5) with easy-plane ($\Delta = 0.5$) and easy-axis ($\Delta = 1.2$) anisotropy (panels e and g respectively). Bottom panels (b, d, f, h): Extracted dynamical exponent $z(L, t, m_{\max})$ by performing curve-fitting inside a sliding window of data points. Superdiffusion is observed at the isotropic SU(2) and SU(3) points of the bilinear-biquadratic $S = 1$ chain while diffusive and ballistic spin dynamics are respectively obtained for the easy-axis and easy-plane ZF model. Additional analyses are available in the supplemental material.

field theory which is integrable [52, 53], while the exact microscopic model is not. This long-time crossover to diffusion could possibly have been anticipated based on previous studies on integrability breaking in $S = 1/2$ quantum spin chains, where the integrability breaking is controlled either by adding a parameter or by going to low temperature [17, 54]. For example, the charge conductivity is finite with broken integrability but diverges as a power-law in inverse temperature or strength of integrability-breaking [54], because of the same kind of long-time crossover observed here. The result of diffusion in the non-integrable $S \geq 1$ Heisenberg chain is further evidence that integrability breaking should be regarded as a "dangerously irrelevant" perturbation to dynamics at long times [55]: even if the breaking is weak and irrelevant at low energy in the renormalization group sense, it can strongly modify the long-time behavior by inducing thermalization. It is worth noting two other recent works mentioning (super)diffusion in the $S = 1$ Heisenberg chain [56, 57], although they could not provide a definitive answer regarding the nature of the spin dynamics.

Even in the classical limit $S \to \infty$, where spin operators in Eq. (3) are replaced by standard unit vectors, identifying whether spin diffusion is normal or anomalous has a long-standing history [58–65]. The issue was settled by doing a systematic finite-size analysis in Ref. 66: As in the quantum cases displayed in Fig. 1, $z \to 2$ is only reached asymptotically at relatively long time. This confirms normal diffusive spreading of spin fluctuations, as expected for a non-integrable model. Interestingly, the spin dynamics of an integrable *classical* spin chain with the same symmetries as the Heisenberg model, known as the Faddeev-Takhtajan model [67–69], has recently been explored [38]. The authors are able to show that the spin transport is superdiffusive with $z = 3/2$, and belongs to the KPZ universality class, just like the quantum spin-1/2 Heisenberg chain. In addition to the isotropic point, easy-plane and easy-axis regimes of the model are also investigated and respectively exhibit ballistic and diffusive spin transport; again, just like the quantum $S = 1/2$ Heisenberg model. This legitimately raises questions of possible universality regarding the spin dynamics depending on the nature of the anisotropy in the model. To address this, we extend the current study to larger spin-S quantum models.

Family of S=1 models.— We first turn our attention to various spin-1 models, starting with the isotropic bilinear-biquadratic Heisenberg chain,

$$\hat{h}_{j,j+1} = \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \pm (\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2 . \qquad (4)$$

The two cases considered, with the $\pm$ sign for the biquadratic term, are both integrable. With the minus sign, the model is known as the SU(2)-invariant Babujian-Takhtajan Hamiltonian [70–72]. Its dynamical spin-spin correlation function (1) as well as the long-time decay exponent z are plotted in Fig. 2 (a, b) and show superdiffusion. This is the first time that anomalous spin dynamics is observed in a quantum magnet besides the spin-1/2 Heisenberg chain, and might hint that something universal is responsible for this behavior in integrable systems, such as the rotation symmetry. This is why the Hamiltonian (4) with a plus sign (known as the Uimin-Lai-Sutherland model [73–75]) is interesting, because it extends the SU(2) symmetry to SU(3), and still demonstrate superdiffusive spin dynamics, see Fig. 2 (c, d). This means that having an integrable SU(2)-symmetric model is not in itself a necessary ingredient to have anomalous diffusion, as pointed out in Ref. 48. This statement will be extended by looking at an integrable SO(5)-symmetric spin-2 chain.

Before that, to investigate the effect of anisotropy, we consider the anisotropic $S = 1$ Zamolodchikov-Fateev (ZF) model [76],

$$\begin{aligned}\hat{h}_{j,j+1} = \quad & S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \left(2\Delta^2 - 1\right) S_j^z S_{j+1}^z \\ & + \ 2\left[\left(S_j^x\right)^2 + \left(S_j^y\right)^2 + \left(2\Delta^2 - 1\right)\left(S_j^z\right)^2\right] \\ & - \sum_{a,b\in[x,y,z]} f_{ab}(\Delta) S_j^a S_{j+1}^a S_j^b S_{j+1}^b, \end{aligned} \tag{5}$$

where $f_{ab} = f_{ba}$, $f_{zz} = 2\Delta^2 - 1$, $f_{xz} = f_{yz} = 2\Delta - 1$ and $f_{ab} = 1$ otherwise. This model is analogous to the quantum spin-1/2 XXZ chain in the sense that it is parametrized by a continuous anisotropy parameter Δ and that it is integrable [77–79]. At the isotropic point $\Delta = 1$, it coincides with the BabujianTakhtajan Hamiltonian (4) previously studied. In presence of easy-axis anisotropy, i.e., $|\Delta| > 1$, we observe diffusive dynamics, as shown in Fig. 2 (e, f) for $\Delta = 1.2$, while for an easy-plane anisotropy $|\Delta| = 0.5 < 1$, dynamics is ballistic. In the later case, ballistic transport is expected as the Mazur bound [15, 80, 81] computed analytically in Ref. 82 establishes a non-vanishing Drude weight for this model.

Overall, the dependence on the spin dynamics (diffusive, ballistic and superdiffusive) on the anisotropy is quite familiar, with identical behavior observed for the spin-1/2 quantum Heisenberg chain [26], the classical Faddeev-Takhtajan model [38] and now the $S = 1$ ZF model. However, an interesting feature at $S = 1$ is that the ZF model also shows superdiffusion in the "easy-plane limit" $\Delta = 0$, see Fig. 3 (a, b). The possibility that the $\Delta = 0$ point in the ZF model is special was previously pointed out [82] on the grounds that it is not forced to have ballistic transport by the conserved quantities that force nonzero Drude weight at other values $0 < |\Delta| < 1$.

Integrable SO(5)-symmetric spin-2 chain.— To confirm the universal nature of superdiffusion in integrable isotropic magnets, we study a generalization of the $S = 1$ bilinear-biquadratic Heisenberg chain (4). It can be written down as a one-parameter family of bilinearbiquadratic Hamiltonians in terms of the SO$(2n + 1)$ generators [83, 84]. Focusing on the $n = 2$ case [85] and using a spin-2 formulation of this model [83, 84, 86], one

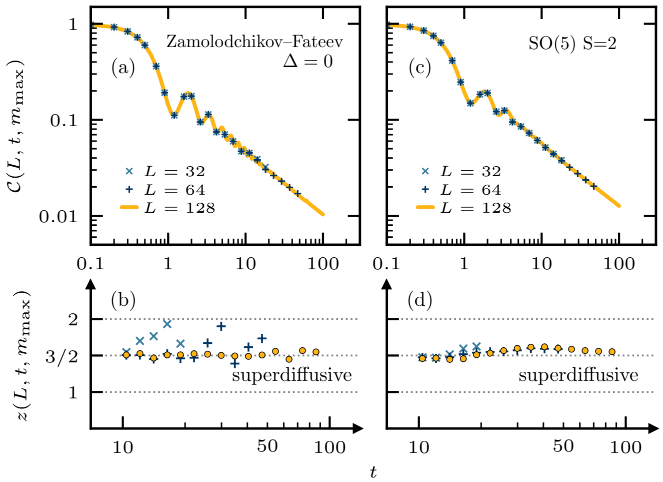

FIG. 3. Top panels (a, c): Infinite temperature spin-spin correlation function (1) for the spin-1 Zamolodchikov-Fateev model (5) at $\Delta = 0$ and the SO(5)-symmetric bilinear-biquadratic $S = 2$ model defined in Eq. (6) for $\theta = \arctan(1/9)$. Bottom panels (b, d): Extracted dynamical exponent $z(L, t, m_{\max})$ by performing curve-fitting inside a sliding window of data points. Superdiffusive spin dynamics is observed in both cases with $z = 3/2$. Additional analyses are available in the supplemental material.

gets,

$$\begin{aligned}\hat{h}_{j,j+1} = \quad & \cos\theta\Big[-1 - \frac{5}{6}\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \frac{1}{9}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\right)^2 \\ & + \frac{1}{18}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\right)^3\Big] + \sin\theta\Big[1 - 5\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \\ & - \frac{17}{12}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\right)^2 + \frac{1}{3}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\right)^3 \\ & + \frac{1}{12}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\right)^4\Big]. \end{aligned} \tag{6}$$

It has an integrable point at $\theta = \arctan(1/9)$, as well as other remarkable points whose values can be generalized as a function of n for all symmetry groups [86–90]. We show in Fig. 3 (c, d) that, once more, anomalous diffusion is present at an integrable and isotropic point which is neither characterized by SU(2), nor SU(3) but SO(5) in this case.

Summary and discussions.— Employing extensive numerical simulations based on tensor network methods, we have investigated the algebraic long-time decay of the infinite temperature spin-spin correlation function in various integrable and non-integrable, isotropic and anisotropic quantum spin-S chains [44]. Our results unequivocally support universal spin dynamics in infinite-temperature one-dimensional magnets, with three different possible regimes: (i) superdiffusive, as in the KPZ universality class, when the model is integrable with extra symmetries such as spin isotropy that drive the Drude weight to zero, (ii) ballistic when the model is integrable with a finite Drude weight, and (iii) diffusive otherwise.

One potential future direction is to demonstrate that the full KPZ [28] scaling function $f_{\rm KPZ}$ is indeed present for all models showing anomalous diffusion, i.e., $\langle S^z_r(t)S^z_0(0)\rangle \sim t^{-2/3} f_{\rm KPZ}[r(\lambda t)^{-2/3}]$ with λ some parameter [91, 92]. As it is very costly to compute the dynamical spin-spin correlation function at all distances r, it would be numerically preferable to use the workaround developed in Ref. 27 for $S = 1/2$ to address this question. An open puzzling question is what ingredient(s) makes the superdiffusive behavior with $z = 3/2$ robust in all isotropic integrable magnets, classical and arbitrary spin-S quantum models alike? It would also be interesting to see if the mechanism of anomalous diffusion proposed in Ref. 29 for the spin-half Heisenberg chain can be extended to all these superdiffusive examples.

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[44] See Supplemental Material at [URL will be inserted by publisher] for details on the convergence with the bond dimension m, on the finite-size effects L and on the effect of width of the fitting window to extract the dynamical exponent z. Moreover, four additional models, not discussed in the main text, are considered in the Supplemental Material. See also Refs. 94, 95, 27, 96 and 97 therein.

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