

Spatiotemporal dynamics of classical and quantum density profiles in low-dimensional spin systems

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We provide a detailed comparison between the dynamics of high-temperature spatiotemporal correlation functions in quantum and classical spin models. In the quantum case, our large-scale numerics are based on the concept of quantum typicality, which exploits the fact that random pure quantum states can faithfully approximate ensemble averages, allowing the simulation of spin-1/2 systems with up to 40 lattice sites. Due to the exponentially growing Hilbert space, we find that for such system sizes even a single random state is sufficient to yield results with extremely low noise that is negligible for most practical purposes. In contrast, a classical analog of typicality is missing. In particular, we demonstrate that, in order to obtain data with a similar level of noise in the classical case, extensive averaging over classical trajectories is required, no matter how large the system size. Focusing on (quasi-)one-dimensional spin chains and ladders, we find a remarkably good agreement between quantum and classical dynamics. This applies not only to cases where both the quantum and classical model are nonintegrable, but also to cases where the quantum spin-1/2 model is integrable and the corresponding classical $s \rightarrow \infty$ model is not. Our analysis is based on the comparison of space-time profiles of the spin and energy correlation functions, where the agreement is found to hold not only in the bulk but also in the tails of the resulting density distribution. The mean-squared displacement of the density profiles reflects the nature of emerging hydrodynamics and is found to exhibit similar scaling for quantum and classical models.

I. INTRODUCTION

Building on seminal results in chaos and random-matrix theory [1, 2] as well as more recent developments such as the eigenstate thermalization hypothesis [3–6], it is now well established that generic quantum and classical many-body systems relax to thermal equilibrium at long times [6–11]. In this context, one of the most generic nonequilibrium situations is given by transport processes of local densities due to a global conservation law [11]. Such transport processes describe the slow relaxation from local to global equilibrium and dominate the late-time and long-wavelength properties of systems with conservation laws. Gaining a deeper understanding how such a macroscopic hydrodynamic behavior emerges from the underlying microscopic equations of motion is the subject of ongoing theoretical research [11, 12], while novel experiments with different quantum-simulator platforms nowadays allow the controlled exploration even of anomalous types of quantum transport and hydrodynamics [13–15]. Key insights have been gained not least due to improved numerical machinery [16–21], as well as the introduction of suitable random-circuit models, which provide minimal models to capture the universal properties of chaotic quantum systems [12, 22–26].

An important role, which can strongly influence the nature of transport in a given model, is played by integrability. On one hand, in the case of classical mechanics, integrability is well defined in terms of the Liouville-Arnold theorem, which requires L (mutually commuting) constants of motion for a system of L spins [27, 28]. The trajectories in such integrable systems remain strictly confined to a small part of phase space, resulting in a breakdown of ergodicity. In contrast, if there are not enough constants of motion, integrability is absent and chaotic dynamics is expected to emerge as a consequence. On the other hand, such a clear-cut definition of integrability is not available in the case of quantum systems [29]. One commonly applied definition is solvability in terms of the Bethe Ansatz, which includes important systems such as the spin-1/2 Heisenberg chain and the one-dimensional Fermi-Hubbard model [30–34]. In particular, for such models it is possible to construct extensive sets of (quasi)local integrals of motion [11, 35, 36], reminiscent of the definition of integrability in classical mechanics. Building on this intricate algebraic structure, much progress in understanding the dynamics of integrable quantum systems has been recently made within the framework of generalized hydrodynamics [37–39], which provides analytical support for early numerical studies [11]. In particular, while integrable systems (due to their coherent quasiparticle excitations) are often expected to exhibit ballistic transport and finite Drude weights [11], the latter indicating that

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induced currents remain (at least partially) conserved on indefinite time scales, it has become clear that the dynamics of integrable systems is much richer. This includes parameter regimes where normal diffusive transport [40, 41], usually associated with chaos, can occur. Moreover, if the integrable model additionally possesses a non-Abelian symmetry, it was found that transport is neither ballistic nor diffusive, but superdiffusive instead [42, 43]. More specifically, it has been argued that this combination of integrability and non-Abelian symmetry generically leads to superdiffusion within the Kardar-Parisi-Zhang (KPZ) universality class with dynamical exponent $z = 3/2$ [11, 43–51], first reported numerically in the case of high-temperature spin transport in the spin-1/2 Heisenberg chain which is $SU(2)$ symmetric [47, 52].

Integrability only accounts for a small region of the full parameter space and is typically found in one-dimensional models. Especially in the case of quantum many-body systems, it appears that integrability is very fragile and even a tiny integrability-breaking perturbation will induce chaos and generic behavior in the limit of large system sizes and long times [6]. Nevertheless, interesting phenomena such as prethermalization can occur in the regime close to integrability [53, 54], and it is an interesting question to what extent the dynamics of weakly perturbed systems can be understood due to their vicinity to an integrable point [55–59]. Generally, however, the vast majority of quantum and classical systems, particularly in spatial dimensions larger than one, are nonintegrable and generic. For such systems, one typically expects that the emerging transport behavior at long times is given by standard diffusion. Such normal diffusive transport has indeed been numerically confirmed in a variety of models [41, 60–65]. However, the numerical extraction of quantitative values for transport coefficients (e.g., diffusion constant), especially in the quantum case, is quite challenging and still an actively pursued direction of research [18, 19, 21]. Furthermore, even in the case of nonintegrable systems which fulfill various indicators of quantum and classical chaos, there still exist counterexamples to the expected diffusive behavior. This includes models with additional symmetries or conservation laws and models with kinetic constraints [25, 66, 67], which can host anomalous types of transport such as subdiffusion, as well as long-range systems where transport can become superdiffusive [68–70].

Even though strongly correlated many-body quantum systems generally do not have an obvious classical limit, a natural choice in the case of quantum spin models is to consider the limit of infinite spin quantum number $s \rightarrow \infty$, where the quantum spin operators become classical three-dimensional vectors. In this context, it is an intriguing question to ask whether and to what extent the dynamics, and in particular the transport properties, of the quantum and the corresponding classical spin model agree with each other. In particular, even though the emerging late-time transport behavior of quantum models may effectively be described by a classical hy-

drodynamic theory (e.g., a diffusion equation), it is not obvious that quantum and classical dynamics agree on a detailed quantitative level (for instance regarding the explicit value of diffusion coefficients). Such a quantitative agreement is nontrivial even at high temperatures, where quantum effects are less pronounced, due to the different microscopic equations of motion. Moreover, sending $s \rightarrow \infty$ can break the integrability of the original spin-1/2 model. Complementing earlier work in this direction [71–73], the goal of this paper is to provide a comprehensive comparison between quantum and classical dynamics in models of interacting spins. To this end, we focus on the buildup of spatiotemporal correlation functions of local spin and energy densities, which probe transport properties in the linear response regime [11], and are also intimately related to experimentally accessible quantities such as the spin structure factor measurable with inelastic neutron scattering [74].

Studying the dynamics of quantum many-body systems is notoriously challenging due to the exponentially growing Hilbert space. In this paper, we rely on the concept of quantum typicality [20, 75], which refers to the fact that even a pure random quantum state can faithfully approximate the full ensemble average. In particular, as we will explain below in more detail, the statistical error of quantum typicality decreases exponentially with the size of the system. As a consequence, significantly less averaging over random states is required in larger systems to obtain the same accuracy. Combined with efficient sparse-matrix techniques for the time evolution of pure quantum states, quantum typicality enables us to simulate spatiotemporal correlation functions in systems with Hilbert-space dimensions far beyond the range of full exact diagonalization. More specifically, we solve the time-dependent Schrödinger equation for models with up to 40 spin-1/2 degrees of freedom, i.e., the total Hilbert space has dimension $2^{40} \approx 10^{12}$, which yields converged results for the buildup of spatiotemporal correlation functions on sufficiently long time scales to extract the asymptotic hydrodynamic behavior. Crucially, we demonstrate that for such enormous Hilbert-space dimensions, the statistical fluctuations of quantum typicality are strongly suppressed, such that even a single random state approximates the spatiotemporal correlation function with an extremely low level of noise that is negligible for all practical purposes. These results are then compared to the corresponding classical system. In contrast to quantum systems, the phase space of classical mechanics only grows linearly with the number of lattice spins, such that simulations are significantly less costly and much larger system sizes can be treated in principle. However, as we demonstrate in this paper, a classical analog of the concept of typicality is missing. In particular, we show that the statistical fluctuations in the classical trajectories are not reduced with increasing system size, such that it remains necessary even for larger and larger systems to perform extensive statistical averaging over a high number of trajectories to achieve the same low noise

level as in the quantum case.

Focusing on (quasi-)one-dimensional spin chains and ladders, we typically find a remarkably good agreement between quantum and classical dynamics. This applies not only to cases where both the quantum and classical model are nonintegrable, but also to cases where the quantum model is integrable and the corresponding classical model is not. Our analysis is based on the comparison of space-time profiles of the spin and energy correlation functions, where the agreement is found to hold not only in the bulk but also in the tails of the resulting density distribution. This fact also manifests itself in the time dependence of the mean-squared displacement of the density profiles, which reflects the nature of emerging hydrodynamics and exhibits very similar scaling for quantum and classical models, at least on the time and length scales considered here, with the exception of cases where transport is dominated by integrability. Furthermore, we show that such a correspondence between quantum and classical dynamics can also be achieved in less obvious cases where the original quantum system is not directly written in spin language. In particular, we consider the one-dimensional Fermi-Hubbard model, which by means of a Jordan-Wigner transform can be brought into the form of a particular type of spin ladder, for which we then take the $s \rightarrow \infty$ limit.

The rest of this paper is structured as follows. In Sec. II, we introduce the quantum spin models, their classical counterparts, as well as the corresponding observables which are studied in this paper. Our numerical approach based on quantum typicality is introduced in Sec. III, where we also explain the methods used to integrate the quantum and classical equations of motion as well as the role of averaging. We present our results for spin and energy transport in Sec. IV, where we consider spin chains in Sec. IV A and spin ladders in Sec. IV B. Moreover, we discuss charge transport in the Fermi-Hubbard chain in Sec. IV C. We summarize our findings and conclude in Sec. V.

II. MODELS AND OBSERVABLES

A. Models

In this paper, we consider different versions of (quasi-)one-dimensional lattice models described by Hamiltonians of the form

$$\mathcal{H} = \sum_{r=1}^L h_r \quad (1)$$

with periodic boundary conditions $L + 1 \equiv 1$. For quantum spin models, the lattice sites are occupied by stationary spins with spin quantum number s , represented by spin vector operators $\mathbf{s}_r = (s_r^x, s_r^y, s_r^z)$. Their components fulfill the defining spin algebra ($\hbar = 1$),

$$[s_r^\mu, s_{r'}^\nu] = i \delta_{rr'} \varepsilon_{\mu\nu\lambda} s_r^\lambda, \quad (2)$$

where $\delta_{rr'}$ is the Kronecker delta, $\varepsilon_{\mu\nu\lambda}$ is the antisymmetric Levi-Civita symbol, and $\mu, \nu, \lambda \in \{x, y, z\}$. For spin quantum number $s = 1/2$, the components can be expressed in terms of Pauli matrices, $s_r^\mu = \sigma_r^\mu / 2$.

First, we consider the anisotropic Heisenberg chain (XXZ chain) with local energy terms

$$h_r = J (s_r^x s_{r+1}^x + s_r^y s_{r+1}^y + \Delta s_r^z s_{r+1}^z) , \quad (3)$$

where $J > 0$ is the antiferromagnetic exchange coupling constant and Δ parametrizes the anisotropy in z direction. For any anisotropy, the total magnetization $S^z = \sum_r s_r^z$ is conserved, $[\mathcal{H}, S^z] = 0$. We note that the spin-1/2 XXZ chain is integrable in terms of the Bethe Ansatz, which has consequences for the transport properties of the model. In particular, the energy current is an exact constant of motion such that energy transport in the spin-1/2 XXZ chain is dissipationless for all values of Δ [11]. Therefore, we here focus on the dynamics of magnetization which can exhibit various types of behavior depending on the choice of Δ , as discussed in detail in Sec. IV A below. On the other hand, when considering the classical version of the XXZ chain with $s \rightarrow \infty$ (cf. Sec. II C), the integrability of the model is broken such that one would naively expect chaotic dynamics resulting in the emergence of diffusive transport. While diffusive energy transport has indeed been found in classical XXZ chains, it turns out that observing clean spin diffusion in all Δ regimes is a subtle issue [76–84]. This might be related to the fact that taking the classical limit $s \rightarrow \infty$ is in some sense only a “weak” integrability-breaking perturbation [59, 85, 86], as it leaves the overall structure (such as the symmetries) of the Hamiltonian intact. As a consequence, the impact of this perturbation on the original quantum dynamics might be less pronounced. As we demonstrate in App. A, observing the onset of standard spin diffusion in classical spin chains (in a Δ regime where quantum dynamics is ballistic) is indeed extremely challenging and requires the analysis of large system sizes on long time scales.

Second, as a quasi-1D spin model, we study the isotropic Heisenberg ladder (XXX ladder),

$$h_r = J \sum_{l=1,2} \mathbf{s}_{r,l} \cdot \mathbf{s}_{r+1,l} + \frac{J}{2} \sum_{r'=r}^{r+1} \mathbf{s}_{r',1} \cdot \mathbf{s}_{r',2} , \quad (4)$$

where the local energy is defined on a “plaquette” consisting of four spins. As above, the total magnetization $S^z = \sum_{r,l} s_{r,l}^z$ is conserved. However, in contrast to the XXZ chain, the XXX ladder is nonintegrable for $s = 1/2$. Thus, this is an example where both the quantum and the classical model are nonintegrable.

Moving deeper into the realm of “genuinely quantum” models, we also consider the Fermi-Hubbard chain with

local Hamiltonians

$$h_r = -t_h \sum_{\sigma=\uparrow,\downarrow} \left(c_{r,\sigma}^\dagger c_{r+1,\sigma} + \text{h.c.} \right) \quad (5)$$

$$+ U \left(n_{r,\uparrow} - \frac{1}{2} \right) \left(n_{r,\downarrow} - \frac{1}{2} \right),$$

where t_h is the hopping amplitude of the spin- σ fermions and U is the on-site interaction strength. The creation operator $c_{r,\sigma}^\dagger$ creates a spin- σ particle at site r , whereas the annihilation operator $c_{r,\sigma}$ annihilates a spin- σ particle at site r . They fulfill the fermionic anticommutation relations,

$$\left\{ c_{r,\sigma}, c_{r',\sigma} \right\} = 0, \quad \left\{ c_{r,\sigma}, c_{r',\sigma}^\dagger \right\} = \delta_{rr'}, \quad (6)$$

and define the local particle number operator $n_{r,\sigma} = c_{r,\sigma}^\dagger c_{r,\sigma}$. Similar to the XXZ chain, the Fermi-Hubbard chain is a prime example of an integrable quantum system. In particular, as in the XXZ chain, energy transport in the Fermi-Hubbard chain is ballistic for all values of U such that we here focus only on charge transport. Notably, by Jordan-Wigner transformation [87], this model is in turn equivalent to a modified version of the spin ladder,

$$h_r = -2J_{\parallel} \sum_{l=1,2} \left(s_{r,l}^x s_{r+1,l}^x + s_{r,l}^y s_{r+1,l}^y \right) \quad (7)$$

$$+ \frac{J_{\perp}}{2} \sum_{r'=r}^{r+1} s_{r',1}^z s_{r',2}^z$$

with $J_{\parallel} = t_h$ and $J_{\perp} = U$. Each leg of the spin ladder is associated with one of the fermionic species \uparrow or \downarrow . The local magnetizations in the spin formulation correspond to occupation numbers in the Hubbard language,

$$n_{r,\sigma} = s_{r,l}^z + \frac{1}{2}. \quad (8)$$

B. Setup and observables

We study the dynamics of local densities ϱ_r of either magnetization (M) or energy (E) based on the time-dependent density-density correlation function,

$$C_{r,r'}(t) = \langle \varrho_r(t) \varrho_{r'} \rangle, \quad (9)$$

where $\langle \bullet \rangle = \text{Tr}[\rho_{\beta} \bullet]$ denotes the expectation value with respect to the canonical density matrix $\rho_{\beta} = \exp(-\beta \mathcal{H})/\mathcal{Z}$ and $\mathcal{Z} = \text{Tr}[\exp(-\beta \mathcal{H})]$ is the canonical partition function at inverse temperature $\beta = 1/k_B T$. Here, operators evolve in time according to the Heisenberg picture, i.e., $\varrho_r(t) = \exp(i\mathcal{H}t) \varrho_r \exp(-i\mathcal{H}t)$.

In the following, we fix $r' = L/2$ and study the time dependence of the profile

$$C_r(t) \equiv C_{r,L/2}(t) = \langle \varrho_r(t) \varrho_{L/2} \rangle. \quad (10)$$

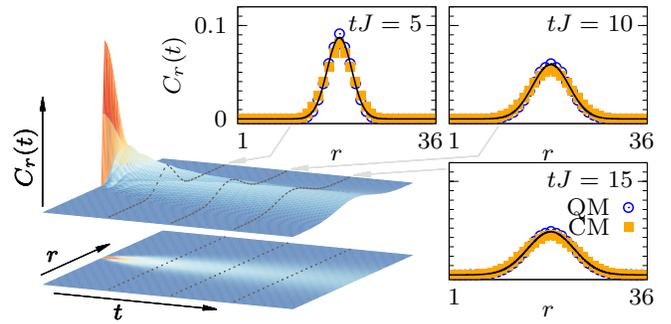


Figure 1. Exemplary plot of an initially peaked density profile that broadens over time by diffusion. The data shows quantum and classical magnetization dynamics in the XXZ spin chain with anisotropy $\Delta = 1.5$ and system size $L = 36$. For a more detailed discussion of the results, see Sec. IV A below. Note that the legend in the lower right panel applies to all other panels.

We focus on the high-temperature limit $\beta \rightarrow 0$, where $\rho_{\beta} \rightarrow 1/d^L$ with Hilbert-space dimension d^L (d denotes the model-specific local Hilbert-space dimension). Accordingly, the density profile is obtained by calculating

$$C_r(t) = \frac{\text{Tr}[\varrho_r(t) \varrho_{L/2}]}{d^L}, \quad (11)$$

where the different local densities, depending on the system's geometry, are defined as

$$\varrho_r^{(M)} = \begin{cases} s_r^z & , \quad \text{XXZ chain} \\ s_{r,1}^z + s_{r,2}^z & , \quad \text{XXX ladder} \end{cases} \quad (12)$$

and

$$\varrho_r^{(E)} = h_r. \quad (13)$$

Moreover, in the case of charge transport in the Fermi-Hubbard chain, we have $\varrho_r = n_{r,\uparrow} + n_{r,\downarrow} - 1 = s_{r,1}^z + s_{r,2}^z$, i.e., analogous to the case of spin dynamics in the XXX ladder.

Initially, a peaked spatial distribution arises for the local magnetizations,

$$C_r^{(M)}(t=0) \begin{cases} \neq 0 & , \quad r = L/2 \\ = 0 & , \quad \text{else} \end{cases}, \quad (14)$$

as can be seen from the spatiotemporal density profiles shown in Fig. 1. A similarly peaked initial density distribution also arises for $C_r^{(E)}(t=0)$, albeit accompanied by two smaller peaks at adjacent lattice sites $L/2 \pm 1$ due to shared bonds between local energy terms h_r and $h_{r\pm 1}$. The main contribution of this work is to provide a detailed comparison between the real-time broadening of such density profiles for quantum and classical spin models.

C. Classical limit

The classical counterpart of the quantum spin models introduced above is achieved by taking the limits of both $\hbar \rightarrow 0$ and $s \rightarrow \infty$ while maintaining the constraint $\hbar\sqrt{s(s+1)} = \text{const}$. Then, the spin operators become three-dimensional vectors of constant length, $|\mathbf{s}_r| = 1$, and the relation (2) turns into

$$\{s_r^\mu, s_{r'}^{\nu'}\} = \delta_{rr'} \varepsilon_{\mu\nu\lambda} s_r^\lambda, \quad (15)$$

where $\{\bullet, \bullet\}$ denotes the Poisson bracket. Consequently, the time evolution of each spin is determined by the Hamiltonian equations of motion,

$$\dot{\mathbf{s}}_r = \{\mathbf{s}_r, \mathcal{H}\} = \frac{\partial \mathcal{H}}{\partial \mathbf{s}_r} \times \mathbf{s}_r. \quad (16)$$

The infinite-temperature correlation function (11) can be obtained in the classical case by taking $\langle \bullet \rangle$ as an average over trajectories in phase space,

$$C_r(t) \approx \frac{1}{N} \sum_{n=1}^N \varrho_r(t) \varrho_{L/2}(0). \quad (17)$$

For each of the $N \gg 1$ realizations, the initial configurations $\mathbf{s}_r(0)$ are drawn at random.

D. Diffusion on a lattice

The correlation functions $C_r(t)$ can be connected to the time dependence of local densities $q_r(t)$ in a scenario, where the initial state is prepared close to the canonical equilibrium density matrix ρ_β as

$$\rho(0) \propto e^{-\beta(\mathcal{H} - \varepsilon \varrho_{L/2})}, \quad (18)$$

which can be expanded in ε and, for high temperatures, takes on the simple form

$$\rho(0) \propto \mathbb{1} + \beta \varepsilon \varrho_{L/2}. \quad (19)$$

For this initial state and using $\text{Tr}[\varrho_r] = 0$,

$$q_r(t) = \langle \varrho_r(t) \rangle = \text{Tr}[\varrho_r(t) \rho(0)] \\ \propto \text{Tr}[\varrho_r(t) \varrho_{L/2}] \propto C_r(t), \quad (20)$$

i.e., $C_r(t)$ describes the dynamics of the local densities $q_r(t)$ after an initial density distribution of the form (14). Speaking differently, $C_r(t)$ can be interpreted as the dynamics and relaxation of some initial spin or energy excitation evolving on top of a featureless infinite-temperature many-body background.

The local densities $q_r(t)$ show diffusive transport, if they fulfill the lattice diffusion equation,

$$\frac{d}{dt} q_r(t) = D [q_{r-1}(t) - 2q_r(t) + q_{r+1}(t)] \quad (21)$$

with some diffusion constant D . The temporal growth of the spatial variance,

$$\Sigma^2(t) = \sum_{r=1}^L r^2 \delta q_r(t) - \left[\sum_{r=1}^L r \delta q_r(t) \right]^2, \quad (22)$$

with $\delta q_r(t) \propto q_r(t)$ normalized to $\sum_r \delta q_r(t) = 1$ for all times t , can also be used for characterizing the dynamics. A scaling according to $\Sigma(t) \propto t^\alpha$ is called *ballistic* for $\alpha = 1$, *superdiffusive* for $1/2 < \alpha < 1$, *diffusive* for $\alpha = 1/2$, *subdiffusive* for $0 < \alpha < 1/2$, and *insulating* for $\alpha = 0$.

Additionally, for initial density distributions of the form (14), the solution of the diffusion equation (21) reads

$$\delta q_r(t) = \exp(-2Dt) I_{r-L/2}(2Dt), \quad (23)$$

where $I_r(t)$ is the modified Bessel function of first kind and of order r . The corresponding spatial dependence for fixed times t is well approximated by Gaussian functions,

$$\delta q_r(t) = \frac{1}{\Sigma(t) \sqrt{2\pi}} \exp\left[-\frac{(r-L/2)^2}{2\Sigma^2(t)}\right], \quad (24)$$

where $\Sigma(t) = 2Dt$. While the scaling analysis of the spatial width (22) may hint at the existence of diffusive transport, the form (24) of the spatial dependence of the density distribution is a precise diagnostics.

III. NUMERICAL METHODS

A. Dynamical quantum typicality

For the quantum systems, we employ the concept of dynamical quantum typicality (DQT) [88–95], which essentially allows us to replace the trace in the calculation of the correlation function (10) by a scalar product between two auxiliary pure states [96, 97],

$$C_r(t) = \langle \phi_\beta(t) | \varrho_r | \varphi_\beta(t) \rangle + \epsilon(|\phi\rangle), \quad (25)$$

where the states

$$|\varphi_\beta(t)\rangle = e^{-i\mathcal{H}t} \varrho_{L/2} |\phi_\beta\rangle, \quad |\phi_\beta(t)\rangle = e^{-i\mathcal{H}t} |\phi_\beta\rangle \quad (26)$$

are constructed with

$$|\phi_\beta\rangle = \frac{\sqrt{\rho_\beta} |\phi\rangle}{\sqrt{\langle \phi | \rho_\beta | \phi \rangle}}. \quad (27)$$

The typical reference state $|\phi\rangle$ is constructed as a random superposition of states $|k\rangle$ in the given orthonormal basis,

$$|\phi\rangle = \sum_{k=1}^{d^L} c_k |k\rangle, \quad (28)$$

where the complex coefficients c_k are randomly drawn from a distribution which is invariant under all unitary transformations in the Hilbert space (Haar measure) [94]. In practice, the real and imaginary parts of the c_k are drawn independently from a standard normal distribution. The variance of the statistical error $\epsilon(|\phi\rangle)$ that arises in Eq. (25) is bounded from above [75],

$$\sigma(\epsilon) < \mathcal{O}\left(\frac{1}{\sqrt{\dim_{\text{eff}}}}\right), \quad (29)$$

where $\dim_{\text{eff}} = \text{Tr}[e^{-\beta(\mathcal{H}-E_0)}]$ with ground-state energy E_0 is the effective Hilbert-space dimension at inverse temperature β . In the infinite-temperature limit, $\lim_{\beta \rightarrow 0} \dim_{\text{eff}} = d^L$, which renders the typicality error negligibly small for the system sizes considered here. Additionally, for $\beta \rightarrow 0$, the calculation of Eq. (25) can be further simplified to [98]

$$C_r(t) = \langle \psi(t) | \varrho_r | \psi(t) \rangle + \epsilon(|\phi\rangle) \quad (30)$$

using just one pure state

$$|\psi(0)\rangle = \frac{\sqrt{\varrho_{L/2} + c} |\phi\rangle}{\sqrt{\langle \phi | \phi \rangle}}, \quad (31)$$

where the constant c ensures that the operator $\varrho_{L/2} + c$ has nonnegative eigenvalues.

The time dependence is now a property of the pure states and can be obtained by iteratively applying the time evolution in small time steps,

$$|\psi(t + \delta t)\rangle = e^{-i\mathcal{H}\delta t} |\psi(t)\rangle, \quad \delta t \ll J. \quad (32)$$

For each time step, the action of the time-evolution operator on the state is obtained by massively parallelized simulations on supercomputers, which rely on both Trotter decompositions [99, 100] and Chebyshev-polynomial expansions [101, 102].

B. Classical averaging

The simulation of the classical spin systems is done by numerically solving the Hamiltonian equations of motion (16) using a fourth-order Runge-Kutta (RK4) scheme. We use a time step δt that is small enough to ensure that the total energy and magnetization are conserved to very high accuracy. The computational complexity of the simulation of classical systems grows only linearly in their system size L and is mainly determined by the number N of samples used in the averaging (17). Importantly, there exists no analog of typicality in classical mechanics, such that we have to average over many samples $N \gg 1$ of independent random initial-state configurations, no matter how large the system size L . This crucial difference between classical and quantum simulations is illustrated in Fig. 2, which shows the single-state trajectories of the equal-site correlation function $C_{L/2}(t)$

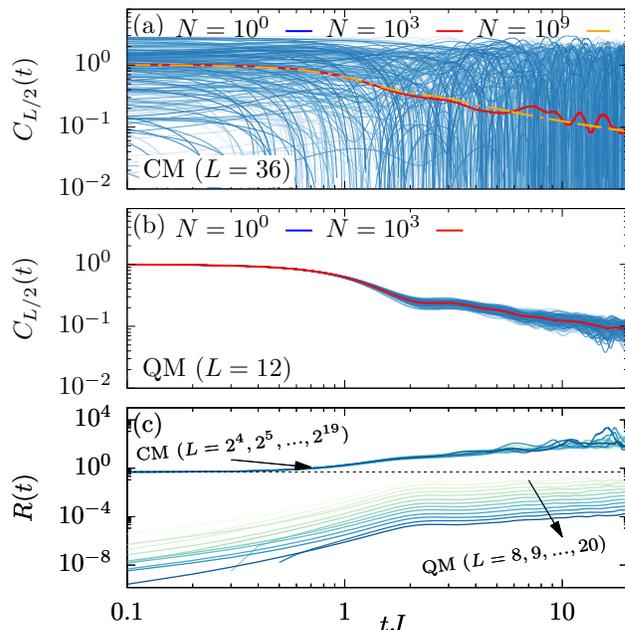


Figure 2. Single-state trajectories of $C_{L/2}(t)$ (blue lines) for 300 random initial states in the XXZ chain with $\Delta = 1.5$ in the classical case (a) and the quantum case (b). Red and orange lines show the corresponding averages over $N = 10^3$ and $N = 10^9$ (only classical) trajectories. (c) Relative variance $R(t)$ of sample-to-sample fluctuations as obtained by Eq. (33) for $N = 10^3$ and different system sizes $L = 2^4, 2^5, \dots, 2^{19}$ (classical) and $L = 8, 9, \dots, 20$ (quantum). Dashed line indicates the value of $R(0)$ for the classical case which is essentially the second moment of the probability distribution for $\varrho_{L/2}^2(0)$ that arises from the random initial configuration of the state. Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that $C_{L/2}(0)$ is set to 1.

for 300 random initial states in the classical [cf. Fig. 2(a)] and the quantum [cf. Fig. 2(b)] version of the XXZ chain with anisotropy $\Delta = 1.5$. In the classical case, each individual trajectory appears random and the behavior of $C_{L/2}(t)$ can only be inferred from the average, whereby the average over $N = 10^3$ trajectories still shows significant deviations from the average over $N = 10^9$ trajectories. In contrast, in the quantum case, the individual random realizations show only small deviations from the average over $N = 10^3$ states, even for the small system size $L = 12$ used here. Fig. 2(c) shows the corresponding relative variance of the sample-to-sample fluctuations,

$$R(t) = \frac{\overline{C_{L/2}(t)^2} - \overline{C_{L/2}(t)}^2}{\overline{C_{L/2}(t)}^2}, \quad (33)$$

for different system sizes $L = 2^4, 2^5, \dots, 2^{19}$ (in the classical case) and $L = 8, 9, \dots, 20$ (in the quantum case). Here, the overbar in $\overline{C_{L/2}(t)}$ denotes the average over $N = 10^3$ samples. Note that a given quantity, here $C_{L/2}(t)$, is sometimes called self-averaging if $R(t)$ decreases with increasing L , e.g., $R(t) \propto L^{-1}$ is referred

to as strong self-averaging in Ref. [103]. As shown in Fig. 2(c), in the classical case, $R(t=0)$ starts at a value that results from the second moment of the probability distribution for the initial value $\varrho_{L/2}^2(0)$. We find that $R(t)$ increases with time, as the average $\overline{C_{L/2}(t)}$ itself decays to smaller and smaller values. Importantly, there is no dependence on system size in this behavior, even for the exponentially increasing L . Thus, self-averaging is absent in the case of classical dynamics such that large values of N are necessary to faithfully capture the ensemble average also for large system sizes L .

In the quantum case, $R(t)$ shows a similar increase in time as above, while at the same time being orders of magnitudes smaller than in the classical case – even for the smallest system size $L = 8$ shown. Crucially, for increasing system size, $R(t)$ decreases exponentially in line with the typicality estimate (29). In this sense, quantum typicality can be seen as an extreme form of self-averaging as exponentially less random realizations are required at larger L to accurately determine the full ensemble average.

IV. RESULTS

The discussion of our numerical results includes the comparison between quantum and classical density dynamics of magnetization in the 1D XXZ chain in Sec. IV A, magnetization and energy in the quasi-1D XXX ladder in Sec. IV B, as well as charge in the Fermi-Hubbard model in Sec. IV C. In all cases, we will focus on time scales where the bulk of the density distribution is still reasonably concentrated around the center and away from the boundaries. The time dependence of the classical correlation functions is always rescaled by the factor $\tilde{s} = \sqrt{s(s+1)}$ to account for the different lengths of quantum and classical spins. For the quantum spin $s = 1/2$ considered here, this factor is $\tilde{s} \approx 0.87$.

A. Magnetization dynamics in the 1D XXZ chain

We first focus on the dynamics of magnetization in the integrable 1D XXZ chain (3) of size $L = 36$ for different values of the anisotropy $\Delta = 0.5, 1$, and 1.5 .

Starting with the anisotropy $\Delta = 1.5$, Fig. 3(a1)-(c2) shows the corresponding profiles $C_r(t)$ from quantum and classical dynamics at fixed times t in linear and semilogarithmic plots. For all values of t , the quantum and the classical profiles show a very good agreement and are accurately described by Gaussian functions (24) that broaden over time. This is in line with the diffusive transport that is expected in the regime $\Delta > 1$ [11]. In order to illustrate the necessity for extensive averaging of the classical data, we show additional data for different sample sizes $N = 2^l \cdot 10^3$ with $l = 0, 1, \dots, 20$ in the same plots. While the time dependence of $C_r(t)$ in the center of the chain is already reasonably well captured for smaller

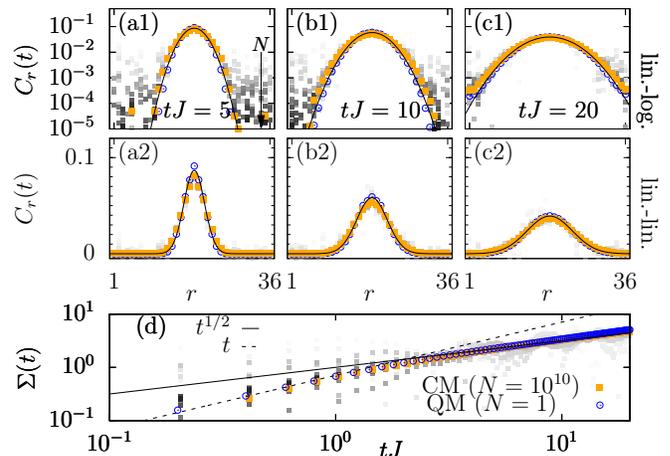


Figure 3. (a1)-(c2) Profiles $C_r(t)$ of magnetization densities in the XXZ spin chain (3) with anisotropy $\Delta = 1.5$ and $L = 36$, sampled over N initial states. Solid lines are Gaussian fits (24) to the QM data. (d) Time-dependent spatial width $\Sigma(t)$ as obtained by Eq. (22). Dashed and solid lines indicate scaling t^α for $\alpha = 1$ and $1/2$. To illustrate the necessity for large sample sizes in the simulations of classical dynamics, additional CM data is shown for different sample sizes $N = 2^l \cdot 10^3$ with $l = 0, 1, \dots, 20$ (grey scales). Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that the legend in panel (d) applies to all other panels.

sample sizes $N = \mathcal{O}(10^3)$, the level of noise away from the center is considerable and only sufficiently suppressed for the largest sample sizes $N = \mathcal{O}(10^9) - \mathcal{O}(10^{10})$. In the following, we will thus always use a rather large sample size $N = 10^9$ for our simulations of classical systems.

In addition to the space-time profiles, Fig. 3(d) shows the time dependence of the corresponding spatial width $\Sigma(t)$ as obtained by Eq. (22). Naturally, an accurate calculation of $\Sigma(t)$ also relies on a good signal-to-noise ratio, which is again illustrated by additional data for smaller sample sizes N in the classical results. For the largest sample sizes, we see a very good agreement between the quantum and the classical results, both in the initial ballistic scaling $\Sigma(t) \propto t$ as well as in the diffusive scaling $\Sigma(t) \propto \sqrt{t}$ for later times. The initial ballistic scaling at short times can be understood as a local expansion of the spin excitation below its mean free path. Above this mean free path, the essentially classical hydrodynamic description applies and the ballistic behavior crosses over to the asymptotic diffusive transport.

Moving on to the isotropic spin chain, Fig. 4 shows analogous data as above, but now for $\Delta = 1.0$. Similarly as before, we see a good agreement between the classical and the quantum results, albeit with some small but visible deviations in the profiles $C_r(t)$ [cf. Fig. 4(a1)-(c2)]. Especially in the tails of the distributions, we find that the overall shape of the profiles is no longer described by Gaussian functions (24), indicating the shift from normal to anomalous diffusion. Indeed, the existence of superdiffusion at the isotropic point is well established (see

Ref. [43] and references therein). More specifically, it has been shown that $C_r(t)$ is well described by the KPZ scaling function, which is similar to a Gaussian in the bulk of the distribution, but exhibits faster than Gaussian decay in the tails. Yet, for the system sizes and times shown here, the agreement with the KPZ scaling function is not fully developed, and the data is rather described by a function $\propto \exp(-a|r - L/2|^3)$. The anomalous transport is also reflected in the scaling of the spatial width $\Sigma \propto t^\alpha$ with $\alpha = 2/3$, which is captured both by the quantum and the classical dynamics [cf. Fig. 4(d)].

As the final comparison in the 1D XXZ chain, Fig. 5 shows data for anisotropy $\Delta = 0.5$. In this regime, the quantum dynamics is dominated by an extensive set of conservation laws and a good agreement between quantum and classical dynamics can no longer be expected. This expectation is confirmed by the space-time profiles $C_r(t)$ [cf. Fig. 5(a1)-(c2)], where we observe noticeable differences between the classical and the quantum results. Interestingly, however, the rough shape of the profiles as well as the overall speed at which they spread over time are captured quite well by the classical results – at least on the time scales shown here. This also pertains to the scaling of the spatial width, $\Sigma(t) \propto t$ [cf. Fig. 5(d)], which indicates the ballistic transport that has been rigorously proven to exist for the quantum system in the thermodynamic limit [35, 36, 105]. However, for longer times $tJ \gtrsim 10$, a slowdown in the scaling of the width $\Sigma(t)$ in the classical data becomes noticeable.

The similarities between the quantum and the classical data in Fig. 5 might indicate that taking the clas-

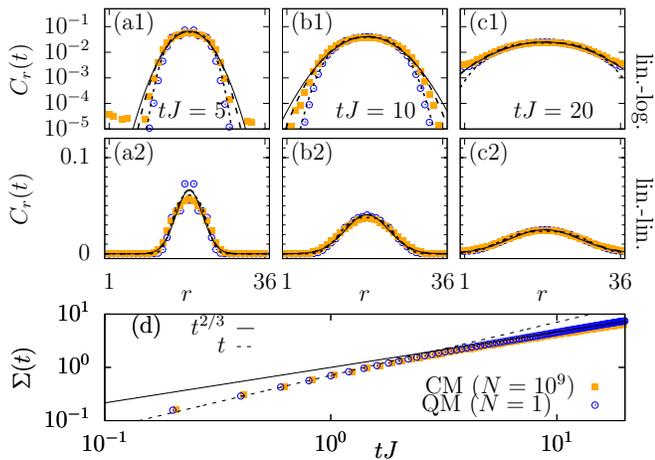


Figure 4. (a1)-(c2) Profiles $C_r(t)$ of magnetization densities in the XXZ spin chain (3) with anisotropy $\Delta = 1.0$ and $L = 36$, sampled over N initial states. Solid lines are Gaussian fits (24) to the QM data. Dashed lines indicate KPZ scaling functions [104]. Dotted lines indicate a function $\propto \exp(-a|r - L/2|^3)$. (d) Time-dependent spatial width $\Sigma(t)$ as obtained by Eq. (22). Dashed and solid lines indicate scaling t^α for $\alpha = 1$ and $2/3$. Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that the legend in panel (d) applies to all other panels.

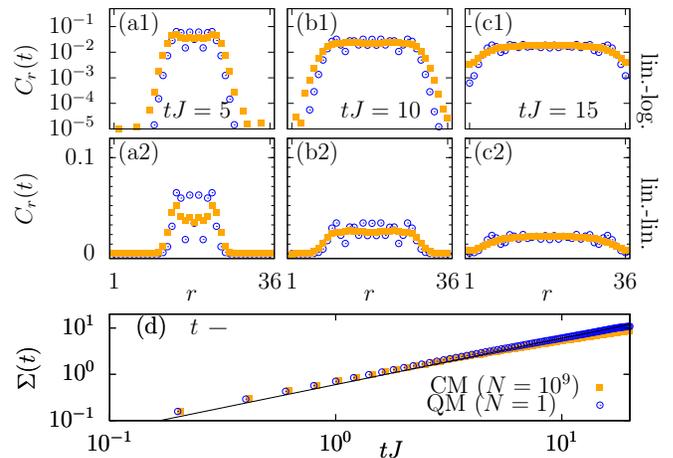


Figure 5. (a1)-(c2) Profiles $C_r(t)$ of magnetization densities in the XXZ spin chain (3) with anisotropy $\Delta = 0.5$ and $L = 36$, sampled over N initial states. (d) Time-dependent spatial width $\Sigma(t)$ as obtained by Eq. (22). Solid line indicates scaling t^α for $\alpha = 1$. Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that the legend in panel (d) applies to all other panels.

sical limit $s \rightarrow \infty$ appears to be a rather weak form of integrability breaking. In particular, while the quantum $s = 1/2$ model features strict ballistic transport, the classical model is expected to be fully chaotic and therefore to exhibit diffusive transport at $\Delta = 0.5$ (especially since we are now away from the potentially special point $\Delta = 1$). However, as becomes clear from Fig. 5, this conjectured diffusive behavior in the classical chain must set in at significantly longer time and length scales. For some additional data from classical dynamics in a larger system of size $L = 2000$, see App. A.

B. Magnetization and energy dynamics in the quasi-1D XXX ladder

Next, we move from 1D chains to quasi-1D spin ladders (4), where the integrability of the quantum system is broken. We compare the quantum and classical dynamics for magnetization and energy in an isotropic spin ladder of length $L = 20$. Note that this corresponds to 40 spin-1/2 lattice sites in total, which is far beyond the range of standard exact diagonalization and close the maximum system sizes that are nowadays in reach of massively parallelized simulations on state-of-the-art supercomputing clusters. The transport of both magnetization and energy in the quantum case $s = 1/2$ is known to be diffusive in this model [60].

Fig. 6 shows the space-time profiles $C_r(t)$ and the spatial width $\Sigma(t)$ for magnetization. Again, the profiles $C_r(t)$ show a very good agreement in the comparison between the quantum and the classical results and are accurately described by Gaussian functions (24). Additionally, the corresponding spatial width $\Sigma(t)$ agrees very

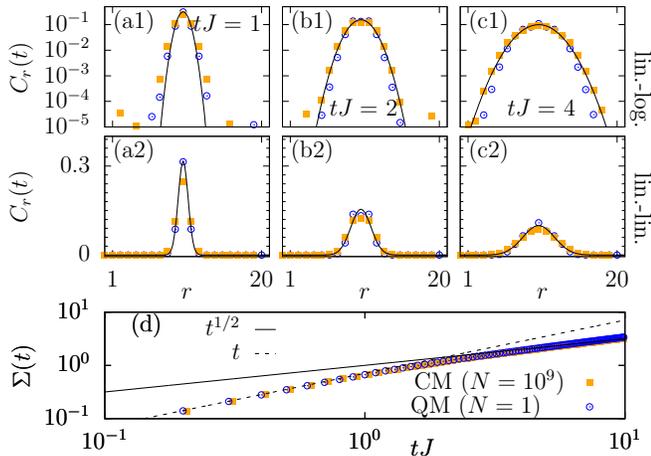


Figure 6. (a1)-(c2) Profiles $C_r(t)$ of magnetization densities in the XXX spin ladder (4) with $L = 20$, sampled over N initial states. Solid lines are Gaussian fits (24) to the QM data. (d) Time-dependent spatial width $\Sigma(t)$ as obtained by Eq. (22). Dashed and solid lines indicate scaling t^α for $\alpha = 1$ and $1/2$. Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that the legend in panel (d) applies to all other panels.

well and the quantum and classical results lie on top of each other, from the initial times of ballistic scaling $\Sigma \propto t$ up to later times of diffusive scaling $\Sigma(t) \propto \sqrt{t}$.

Fig. 7 shows the same data as Fig. 6, but for the dynamics of local energy. The quantum and classical results again agree very well and match the typical signatures of diffusive transport. The only difference compared to the results in Fig. 6 lies in the initial scaling of the spatial width $\Sigma(t)$, which, owing to the broader initial peak for local energy densities, does start at a nonzero initial value.

The good agreement between quantum and classical dynamics in the XXX ladder might not be entirely surprising due to the fact that we are considering high temperatures $\beta \rightarrow 0$ and that both the quantum and the classical model are nonintegrable. However, we still find it remarkable that $C_r(t)$ agrees quantitatively on a very detailed level, leading to an essentially indistinguishable dynamics of the mean-squared displacement $\Sigma(t)$. Crucially, the latter is directly related to physically important quantities such as the diffusion coefficient. Our results in Figs. 6 and 7 suggest that this diffusion coefficient is the same in the quantum and the classical model, emphasizing that (the significantly less costly) simulations of classical systems can provide a useful strategy to gain insights into the properties of strongly correlated quantum many-body systems. While not shown here, we expect a similarly good agreement between quantum and classical dynamics also for XXZ spin ladders [i.e., when incorporating an anisotropy Δ in the Hamiltonian (4)]. In particular, studying the equal-site correlation functions $C_{L/2}(t)$ of magnetization and energy, [72] found a convincing agreement between the quantum and classical

dynamics in ladders with $\Delta = 0.5, 1$, and 1.5 .

C. Charge dynamics in the Fermi-Hubbard chain

Finally, we turn to the dynamics of local charge densities in the integrable Fermi-Hubbard chain, where earlier numerical studies have found clear signatures of diffusive charge dynamics for strong interactions $U/t_h \approx 16$ [41, 106]. However, let us note that this observation of diffusion is at odds with generalized hydrodynamics results, which predict the occurrence of superdiffusive charge transport [11], given the $SU(2)$ symmetry of the Fermi-Hubbard model (similar to the case of spin transport in the isotropic spin-1/2 Heisenberg chain). Here, we consider a somewhat lower interaction strength, $U/t_h = 4$, and study chains of length $L = 18$. Let us stress again that, while the Fermi-Hubbard chain has no obvious classical limit, the Jordan-Wigner transformation in Eq. (7) and the subsequent limit $s \rightarrow \infty$ allows for a comparison with classical dynamics also in this case.

Fig. 8 shows the corresponding space-time profiles $C_r(t)$ and the spatial width $\Sigma(t)$. Comparing the results for the quantum and the classical dynamics, we see a good agreement in the space-time profiles for all values of t shown here. While the profiles are well described by Gaussians (24) in the bulk of the system, we observe notable deviations from these Gaussian fits in the tails of the distributions [cf. Fig. 8(b1)]. This might be reminiscent of the superdiffusive KPZ scaling of spin transport in the Heisenberg chain discussed above in Fig. 4. Then again, the overall broadening of the profiles seems to follow a diffusive scaling, $\Sigma(t) \propto \sqrt{t}$ [cf. Fig. 8(d)], both for

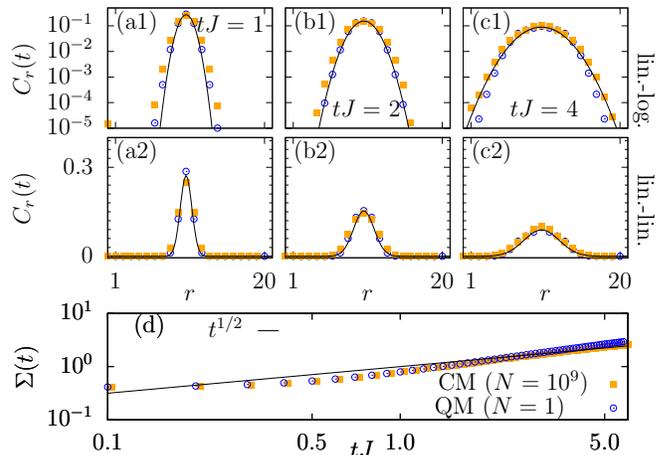


Figure 7. (a1)-(c2) Profiles $C_r(t)$ of energy densities in the XXX spin ladder (4) with $L = 20$, sampled over N initial states. Solid lines are Gaussian fits (24) to the QM data. (d) Time-dependent spatial width $\Sigma(t)$ as obtained by Eq. (22). Solid line indicates scaling t^α for $\alpha = 1/2$. Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that the legend in panel (d) applies to all other panels.

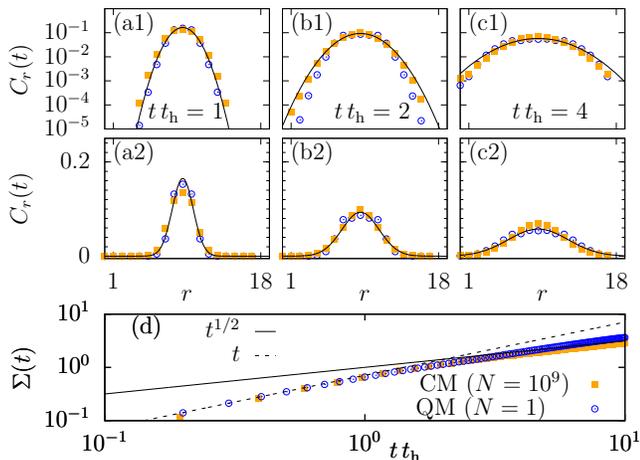


Figure 8. (a1)-(c2) Profiles $C_r(t)$ of charge densities in the Fermi-Hubbard chain (5) with $L = 18$ and $U/t_h = 4$, sampled over N initial states. Solid lines are Gaussian fits (24) to the QM data. (d) Time-dependent spatial width $\Sigma(t)$ as obtained by Eq. (22). Dashed and solid lines indicate scaling t^α for $\alpha = 1$ and $1/2$. Note that we consider the high-temperature limit $\beta \rightarrow 0$ and that the legend in panel (d) applies to all other panels.

quantum and classical dynamics. To be more precise, at the longest time $tt_h = 10$ shown in Fig. 8(d), we actually do observe some slight deviations in the time dependence of $\Sigma(t)$, where the broadening in the classical case becomes notably slower compared to the quantum case. This observation might hint at the possibility that the nonintegrable classical model supports diffusion, while the original integrable Fermi-Hubbard chain asymptotically shows a crossover to superdiffusion. However, resolving the latter is numerically quite challenging.

Finally, we note that the remarkable agreement between quantum and classical dynamics observed for $U/t_h = 4$ in Fig. 8 can in general neither be expected for very small interactions $U/t_h \rightarrow 0$ nor for much stronger interactions. On the one hand, for weak interactions, the charge dynamics becomes more and more ballistic, as the model is approaching the limit of free fermions. On the other hand, for much stronger values of U , the on-site interaction dominates the dynamics and reduces the effective number of interacting neighbors in the system [107], which is expected to affect the comparability between quantum and classical dynamics.

V. CONCLUSION

In this paper, we have compared the quantum and classical dynamics of spatiotemporal density-density correlation functions in different (quasi-)one-dimensional systems for high temperatures $T \rightarrow \infty$. In the quantum case, we employed the concept of quantum typicality in combination with an efficient forward propagation of pure states to obtain results in spin-1/2 systems with up to

40 lattice sites with an extremely low level of statistical noise. In order to achieve a similar signal-to-noise ratio in the classical case, we performed extensive averaging over large samples of $N = \mathcal{O}(10^9) - \mathcal{O}(10^{10})$ classical trajectories. Based on the comparison of space-time profiles of spin and energy correlations, we found a remarkably good agreement between quantum and classical dynamics – not only in cases where both the quantum and classical model are nonintegrable, but also in cases where the quantum spin-1/2 model is integrable and the corresponding classical $s \rightarrow \infty$ model is not. Further, we found that this agreement not only holds in the bulk but also in the tails of the density distributions. The good agreement between quantum and classical results also manifested itself in the time dependence of the mean-squared displacement of the density profiles, which exhibited very similar scaling for quantum and classical models, at least on the time and length scales considered here.

Furthermore, we showed that such a correspondence between quantum and classical dynamics can also be achieved in less obvious cases where the original quantum system is not directly written in spin language. In particular, we considered the one-dimensional Fermi-Hubbard model, which by means of a Jordan-Wigner transform can be brought into the form of a particular type of spin ladder, for which we then take the $s \rightarrow \infty$ limit. The results from the simulations of quantum and classical dynamics showed a good agreement, both for the space-time profiles of local charge as well as the time dependence of the corresponding spatial width, at least for the interaction strength considered here. This agreement is expected to break down for smaller interaction strengths, where the Fermi-Hubbard model approaches the integrable limit of free particles, as well as for much stronger interaction strengths, where the effective number of interacting neighbors per site is reduced significantly [107].

There are several future directions of research to explore. Apart from the question how far the agreement between quantum and classical dynamics carries over to finite temperatures, it would also be interesting to further explore the Fermi-Hubbard model in more detail. For instance, one might expect that the agreement between quantum and classical dynamics increases in the extended Fermi-Hubbard model, where additional interactions increase the effective number of interacting neighbors. Moreover a study in higher spatial dimensions would be interesting, where the range of the simulation of quantum systems is severely limited.

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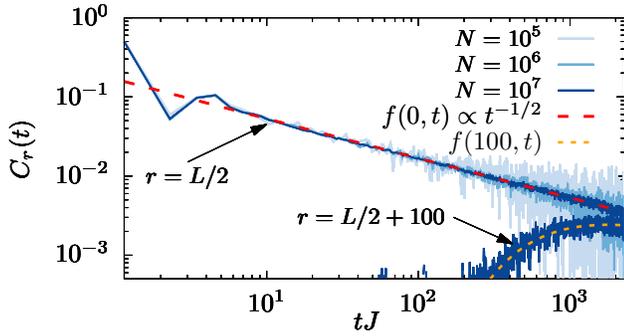


Figure 9. Classical dynamics of $C_r(t)$ for $r = L/2$ and $r = L/2 + 100$ in a XXZ spin chain with anisotropy $\Delta = 0.5$ and large system size $L = 2000$. Dashed lines indicate a Gaussian fit to the equal-site correlation function $C_{L/2}(t)$ [cf. Eq. (A1)]. Note that we consider the high-temperature limit $\beta \rightarrow 0$.

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Appendix A: Large classical XXZ chain with $\Delta = 0.5$

Complementary to the results for the XXZ chain with anisotropy $\Delta = 0.5$ discussed in Sec. IV A, we here present additional classical results for longer times and a

significantly larger chain of size $L = 2000$.

Fig. 9 shows the corresponding dynamics of the equal-site correlation function $C_{L/2}(t)$ for different sample sizes $N = \mathcal{O}(10^5) - \mathcal{O}(10^6)$. For the largest sample size shown, a diffusive decay $C_{L/2}(t) \propto t^{-\alpha}$ with $\alpha = 1/2$ becomes visible on longer time scales, which follows from the Gaussian profile [cf. Eq. (24)]

$$f(\tilde{r}, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{\tilde{r}^2}{4Dt}\right), \quad \tilde{r} = r - L/2 \quad (\text{A1})$$

where the diffusion constant D may serve as a single fit parameter. In addition to the data for $C_{L/2}(t)$, we also show the correlation function $C_r(t)$ at a site $r = L/2 + 100$ far away from the center of the chain, where $C_r(t)$ starts in the initial infinite-temperature many-body background and increases at times when the density peak in the center of the chain has spread sufficiently far over the system. Remarkably, despite the considerable fluctuations that are still present for the shown sample size, the time dependence of $C_r(t)$ appears to be well captured by the function (A1). Note that we do not perform another fit, but instead reuse the diffusion constant D obtained in the fit to $C_{L/2}(t)$.

However, a genuine confirmation of diffusion would again require the study of the full spatial dependence of the density distributions $C_r(t)$. This in turn necessitates a substantially larger sample size N , which, given the combination with large L and long time scales, remains numerically challenging. A more instructive approach to the transport behavior in larger systems might be to study the density dynamics in momentum space, i.e., the decay of long-wavelength Fourier modes of the real-space data $C_r(t)$, for a different class of initial states [108].

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