Real-time broadening of bath-induced density profiles from closed-system correlation functions

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The Lindblad master equation is one of the main approaches to open quantum systems. While it has been widely applied in the context of condensed matter systems to study properties of steady states in the limit of long times, the actual route to such steady states has attracted less attention yet. Here, we investigate the nonequilibrium dynamics of spin chains with a local coupling to a single Lindblad bath and analyze the transport properties of the induced magnetization. Combining typicality and equilibration arguments with stochastic unraveling, we unveil for the case of weak driving that the dynamics in the open system can be constructed on the basis of correlation functions in the closed system, which establishes a connection between the Lindblad approach and linear response theory at finite times. In this way, we provide a particular example where closed and open approaches to quantum transport agree strictly. We demonstrate this fact numerically for the spin-1/2 XXZ chain at the isotropic point and in the easy-axis regime, where superdiffusive and diffusive scaling is observed, respectively.

I. INTRODUCTION

Understanding the dynamics of many-body quantum systems has seen remarkable progress in recent years [1], including the origin of thermalization and hydrodynamics under unitary time evolution [2–5], the possibility of weak and strong forms of ergodicity breaking [6, 7], and the emergence of universality far from equilibrium [8–12]. In addition to theoretical breakthroughs, these and related areas have also profited immensely from experiments like seminal quantum simulators, where both closed and open systems can be probed [13–15]. The competition of internal quantum dynamics, dissipation, and external driving opens up a vast landscape of exotic nonequilibrium phenomena [16, 17].

In systems with a conservation law, e.g., spin models with conserved total magnetization, a key role is played by the slow relaxation of the corresponding hydrodynamic modes [18]. While chaotic systems are typically expected to exhibit diffusion [19–21], anomalous transport can occur, e.g., in the presence of long-range interactions [22–24], in disordered and kinetically constrained systems [25–27], or in the case of integrable models [28]. For the latter, the concept of generalized hydrodynamics provides a powerful framework to predict the emerging transport behavior [29, 30]. In generic systems, in contrast, extracting quantitative values of transport coefficients like diffusion constants remains a formidable challenge even for sophisticated numerical techniques [31–34].

![FIG. 1.](image)

A canonical approach to quantum transport in closed spin or Hubbard type models is given by linear response theory (LRT) in the form of equilibrium correlation functions [18]. A number of efficient numerical methods have been used to evaluate such correlation functions either in real time or in the frequency domain, including exact diagonalization [35], matrix product state techniques...
[36, 37], Lanczos methods [38], dynamical quantum typicality [39–43], semiclassical approximations [44], or quantum Monte Carlo [45].

An alternative approach to transport is to consider an open-system setting, where the model is connected at its ends to reservoirs, which drive a current through the bulk [46–49]. The time evolution is often described by a Lindblad master equation which induces a nonequilibrium steady state at long times. State-of-the-art algorithms to solve the Lindblad equation are based on a matrix-product-operator formulation, which gives access to huge system sizes, e.g., on the order of hundreds of spin-1/2 degrees of freedom [50–54]. Especially for systems in the thermodynamic limit, it is expected that the specific form and strength of the system-bath coupling become irrelevant for the steady state. However, the involved Lindblad operators in practice often have to be chosen heuristically. Moreover, extra care has to be taken in the case of finite systems to reproduce the correct behavior of the actual closed system of interest [55]. While agreement between boundary-driven transport and LRT has numerically been observed for selected examples [56, 57], there is no general proof that both approaches need to agree [18, 58–61], also at weak driving.

In this Letter, we make a significant step forward to bridge the conceptual gap between closed-system and open-system numerical approaches to quantum transport. Focusing on the case of weak driving and relying on typicality and equilibration arguments, we establish a connection between LRT and the finite-time dynamics of an open quantum system in a simple setting introduced below and sketched in Fig. 1(a). Specifically, we unveil that open-system dynamics can be constructed from closed-system correlation functions. This novel connection entails both physical implications regarding the transport properties and consequences regarding efficient numerical simulations of open systems. We also note that Green-Kubo type relations connecting equilibrium correlation functions to open-system transport have been obtained before in classical systems, see e.g., Refs. [58, 62]. We stress that our results and our framework are distinct from such approaches. Rather we provide a means to understand individual trajectories in the unraveling of Lindblad master equations from the dynamics of the closed system.

II. SETUP

While our theoretical framework applies more generally to other systems, we here demonstrate its validity for the spin-1/2 XXZ chain as a timely example,

$$H = J \sum_{r=1}^{N} (S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z),$$

where $S_r^x, y, z$ are spin-1/2 operators at site $r$, $J > 0$ is the antiferromagnetic coupling constant, $\Delta$ denotes the anisotropy in $z$ direction, and $S_{N+1}^z = S_1^z$. The high-temperature spin-transport properties of the integrable XXZ chain have been in the focus of intense theoretical and experimental efforts in recent years. While normal diffusion emerges for $\Delta > 1$ [18], transport is superdiffusive at $\Delta = 1$ with spatiotemporal correlations following the Kardar-Parisi-Zhang (KPZ) scaling function (see e.g. [28, 37, 63, 64]).

In this Letter, we consider a nonequilibrium situation, where the system of interest is coupled to an external bath, as described by the Lindblad equation

$$\dot{\rho}(t) = \mathcal{L}[\rho(t)] = i[\rho(t), H] + \mathcal{D}[\rho(t)],$$

which consists of a coherent time evolution of the density matrix $\rho(t)$ and an incoherent damping term

$$\mathcal{D}[\rho(t)] = \sum_j \alpha_j \{ L_j \rho(t) L_j^\dagger - \frac{1}{2} [\rho(t), L_j^\dagger L_j] \},$$

with non-negative rates $\alpha_j$. Lindblad operators $L_j$, and the anticommutator $\{ \cdot, \cdot \}$. While the derivation of Eqs. (2) and (3) can be a subtle task for a given microscopic model [47, 65] (and might not always be justified [66, 67]), it is the most general form of a time-local quantum master equation, which maps a density matrix to a density matrix [68]. Here, we focus on arguably the simplest possible setup, see Fig. 1(a), where $H$ is coupled to the bath at a single lattice site,

$$L_1 = S_r^+, \quad \alpha_1 = \gamma(1 + \mu),$$

$$L_2 = L_1^\dagger = S_r^-, \quad \alpha_2 = \gamma(1 - \mu),$$

where $\gamma$ is the system-bath coupling, $\mu$ is the driving strength, and $L_1$ and $L_2$ are local Lindblad operators at site $r_0 = N/2$. (This site is arbitrary due to periodic boundaries). Note that throughout our work and consistent with the literature on transport [18], we refer to the influence of Lindblad operators as driving. This type of incoherent driving should not be confused with a coherent driving by a time-dependent Hamiltonian.

Considering a homogeneous initial state $\rho(0)$ and choosing $\mu > 0$, excess magnetization is induced at the bath site and then transported through the chain. Specifically, we study the time evolution of local densities $\langle S_r^z(t) \rangle = \text{tr}[\rho(t) S_r^z]$, see Fig. 1(b), which depends on the parameters of the system $H$, but also on the bath parameters $\gamma$ and $\mu$. The emerging transport behavior reflects itself in the growth of the spatial variance [18]

$$\Sigma_r^2(t) = \sum_r \langle S_r^z(t) \rangle^2 - \left[ \sum_r \langle S_r^z(t) \rangle \right]^2,$$

with $\langle S_r^z(t) \rangle = \sum_r \langle S_r^z(t) \rangle$. Importantly, as shown in Fig. 1(c), we find that at weak driving $\mu = 0.1 \ll 1$, the transport behavior of the isolated XXZ chain carries over to the behavior of the open system with diffusive scaling ($\Sigma^2(t) \propto t$) at $\Delta = 1.5$ and superdiffusive KPZ scaling ($\Sigma^2(t) \propto t^{4/3}$) at $\Delta = 1.0$. A key contribution of the
present work is to show how this result can be understood by connecting the Lindblad setting to the dynamics of correlation functions in the closed system.

III. TRAJECTORIES AND WEAK LINDBLAD DRIVING

One possibility to solve the Lindblad equation is given by the concept of stochastic unraveling, which relies on pure states $|\psi\rangle$ rather than density matrices [69, 70]. It consists of an alternating sequence of stochastic jumps and deterministic evolutions with respect to an effective Hamiltonian $H_{\text{eff}} = H - (i/2) \sum_j \alpha_j L_j^\dagger L_j$. Given Eqs. (4) and (5), $H_{\text{eff}}$ here takes on the form

$$H_{\text{eff}} = H - \frac{i}{2} \gamma (1 + \mu) + i \gamma \mu r_0 \approx H - \frac{i}{2} \gamma,$$  

where $r_0 = S^{+}_z S^{-}_z = S_z^2 + 1/2$, and the approximation in the last step applies for weak driving $\mu \ll 1$. In particular, for $\mu \ll 1$, the deterministic evolution $\exp(-iH_{\text{eff}}t)\ket{\psi(0)}$ simplifies,

$$\ket{\psi(t)} \approx e^{-\gamma t/2} e^{-iHt} \ket{\psi(0)},$$  

i.e., apart from the scalar damping term, the dynamics is generated by the closed system $H$ only. This simplification will be central to derive our analytical prediction below. However, in our numerical simulations, we always take into account the full expression of $H_{\text{eff}}$ for the stochastic unraveling without approximation.

IV. DYNAMICAL TYPICALITY

In a nutshell, quantum typicality asserts that a random pure quantum state can faithfully reproduce properties of the full statistical ensemble [71–75]. For instance, a homogeneous magnetization distribution at $t = 0$, cf. Fig. 1(b), can be readily realized by a Haar-random initial state $\ket{\psi(0)}$ as

$$\ket{\psi(0)} = \sum_{\phi_j} (a_j + ib_j) \ket{\phi_j},$$  

where the coefficients $a_j$ and $b_j$ in some basis $\ket{\phi_j}$ are drawn at random from a Gaussian distribution with zero mean, and $\ket{\psi(0)}$ mimics the maximally mixed state $\rho \propto 1$ [71–75]. It is further instructive to consider, for the moment, an artificial scenario with a quantum jump immediately at $t = 0$, i.e., $\ket{\psi(0)} \rightarrow \ket{\psi'} \propto L_1 \ket{\psi(0)}$. This results in a random
superposition over a subset of pure states with a spin-up at \( r_0 = N/2 \), which mimics \( \rho \approx 1 + S_z^{r_0} \). Then, the deterministic evolution \( d_r(t) \) at weak driving, cf. Eq. (8),

\[
d_r(t) = \frac{\langle \psi'(t)|S_z^r|\psi'(t)\rangle}{\|\psi'(t)\|^2} \approx \langle \psi'|e^{iHt}S_z^r e^{-iHt}|\psi'\rangle,
\]

can be rewritten as \( d_r(t)/2 = \langle S_z^r(t)S_z^{r_0}(0) \rangle \) via typicality, with \( S_z^r(t) = e^{iHt}S_z^r e^{-iHt} \), and \( \Theta = \text{tr}\cdot/2^N \) denoting the infinite-temperature average \[76]. Thus, the dynamics of expectation values \( d_r(t) \) during the deterministic process are generated by equilibrium correlation functions of the closed system \( H \). We numerically demonstrate the validity of this finding in a test setting, where we consider for simplicity only the single jump operator \( L_1 \) and artificially fix the jump times to \( \tau_k = k\delta \tau \) with \( \delta \tau = 10 \). As shown in Fig. 2(a), \( \langle S_z^r(t)S_z^{r_0}(0) \rangle \) indeed reproduces the deterministic dynamics after the first and before the next jump, \( 0 < t < 10 \). Furthermore, Fig. 2(a) already highlights that we can actually predict open-system trajectories even with many jumps, which is a main result of this work. As explained in the following, such a description of trajectories with multiple jumps is achieved by superimposing closed-system correlation functions \( \langle S_z^r(t)S_z^{r_0}(0) \rangle \) appropriately. We should stress that the accuracy of the typicality approximation used so far increases exponentially with \( N \) \[76].

V. CONNECTING LRT AND QUANTUM TRAJECTORIES

To proceed, we now take into account also the jump operator \( L_2 \), but still use jump times \( \tau_k = k\delta \tau \) for illustration. Averaging over trajectories weighted according to the jump probabilities of \( L_1 \) and \( L_2 \) with their different prefactors \( \gamma(1+\mu) \) and \( \gamma(1-\mu) \), cf. text above Eq. (9), one finds \( d_r(t)/2 = \mu \langle S_z^r(t)S_z^{r_0}(0) \rangle \) for the initial time evolution after the first jump, \( 0 < t < 10 \), see Fig. 2(b). While this idealized prediction cannot hold exactly at later stages of the trajectory, one can make further progress by assuming a sufficiently small value of \( \gamma \). Then, within the deterministic evolution, the system has enough time to equilibrate and expectation values approach \( d_r(t)/2 = \mu \langle S_z^r(0)^2 \rangle /N \) [cf. Fig. 2(b)], which approaches zero for large \( N \) and thus becomes close to the local magnetizations before the initial jump at \( t = 0 \). Eventually, another jump must occur at some time \( \tau \), and, given the above equilibration, a reasonable expectation for the subsequent deterministic evolution is \( d_r(t)/2 = \mu \langle S_z^r(0)^2 \rangle /N + \mu - \mu/N \langle S_z^r(t-\tau)S_z^{r_0}(0) \rangle \). Reiterating this procedure, we end up with a prediction for the entire trajectory with jump times \( \tau_k \),

\[
a_k = \frac{A_k}{\mu} \Theta(t - \tau_k) \langle S_z^r(t - \tau_k)S_z^{r_0}(0) \rangle,
\]

where \( \Theta \) is the Heavyside function. The amplitudes \( A_k \) read \( A_k/2 = \frac{1}{2} - \bar{d}_{r_0}(\tau_k - 0^+) /\mu \) and measure the remaining deviation from the long-time equilibrium value, with \( \bar{d}_{r_0} \) given by Eq. (8).

\[
a_k = \frac{\mu - 2\bar{d}_{r_0}(\tau_k - 0^+)}{2 - 4\mu \bar{d}_{r_0}(\tau_k - 0^+)},
\]

with \( A_k \rightarrow 1 \) if \( \bar{d}_{r_0}(\tau_k - 0^+) \rightarrow 0 \). In our numerics, we find Eqs. (11) and (12) to be well fulfilled even if full equilibration is not reached, see Fig. 2(b). Importantly, Eq. (11) not only applies at the bath site \( r_0 = N/2 \), but actually describes the full site dependence \( \bar{d}_r(t) \) accurately, see Fig. 3, albeit with slight deviations at later times.

VI. FROM WEAK TO STRONG DRIVING

While we have chosen artificial \( \tau_k \) in Figs. 2 and 3 for illustrative reasons, we now turn to the actual solution of the Lindblad equation. Our analytical prediction for \( \langle S_z^r(t) \rangle \) follows from averaging Eq. (11) over trajectories with random jump times \( (\tau_1, \tau_2, \ldots) \), i.e.,

\[
\langle S_z^r(t) \rangle \approx \langle 1/T_{\text{max}} \rangle \sum T \bar{d}_r(T)(t).
\]

Specifically, given the
exponential damping in Eq. (8) for $\mu \ll 1$, the $\tau_k$ are given by $\tau_{k+1} = \tau_k - \ln \varepsilon / \gamma_1$, where a new $\varepsilon$ is drawn at random from $[0, 1]$ after each jump. Hence, if the correlation function $\langle S_z^1(t)S_z^0(0) \rangle$ is known, it is rather straightforward to construct the prediction (11) and the average numerically. Crucially, the computational costs of this procedure are significantly lower compared to the full stochastic unraveling such that we are able to generate dynamics for system sizes $N = 36$, see Fig. 4 and Appendix B, which is approximately the maximum size reachable for typicality-based calculations of correlation functions. Note, however, that even larger system sizes might be reached when calculating correlation functions from matrix-product state techniques.

In Fig. 4(a)-(c), we summarize our numerical results for $\langle S_z^2(t) \rangle$, where we consider (i) weak driving $\mu = 0.1$ and weak coupling $\gamma/J = 0.1$, (ii) strong coupling $\gamma/J = 1$, and (iii) strong driving $\mu = 1$. We compare our prediction to the numerically exact stochastic unraveling which is performed for the full $H_{\text{eff}}$ and a homogeneous initial state. We find that the prediction and the exact dynamics agree perfectly for (i), while the agreement becomes worse for (ii) and (iii), as expected. The convincing agreement in Fig. 4(a) confirms our initial observation that the transport behavior of the closed system carries over to the open system (cf. Fig. 1). Specifically, superpositions of correlation functions with diffusive (superdiffusive) scaling at $\Delta = 1.5$ ($\Delta = 1$) according to Eq. (11) yield a dynamics with the same scaling, see also Appendix D.

 VII. CONCLUSION

In summary, we have studied nonequilibrium dynamics and transport in spin chains with a local coupling to a Lindblad bath. For weak driving, we have unveiled that the open-system dynamics can be constructed on the basis of closed-system correlation functions, which establishes a connection between LRT and the Lindblad setting. For this specific setting, from a conceptual point of view, our results confirm the common assumption that closed-system and open-system approaches to transport should agree if the relevant parameters are chosen appropriately. From a practical point of view, our framework sheds new light on the efficient stochastic unravelings of Lindblad equations for large system sizes and long time scales. While we have chosen the XXZ chain as a timely example, our framework can be applied also to other spin or Hubbard models.

Promising directions of future research are, e.g., the generalization of our results to boundary-driven situations with a bath at each end of the system, which seems to be feasible [77]. Another interesting avenue is to study the role of integrability in more detail. In particular, our finding of persisting superdiffusive transport even in the presence of a system-bath coupling appears related to recent works that explored effect of weak integrability-breaking perturbations [78, 79].

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Appendix A: Amplitudes

One possibility to derive the amplitudes in Eq. (12) is based on typicality arguments. To this end, consider a maximally random pure state $|\psi(\tau_j - \tau^+)\rangle$ under the constraint

$$d_{\tau_0}(\tau_j - \tau^+) = x,$$

(A1)

before a jump occurs at time $\tau_j$. Then, we have

$$y_1 = \|L_1|\psi(\tau_j - \tau^+)\|_2^2 = \frac{1}{2} - x \quad \text{(A2)}$$

and

$$y_2 = \|L_2|\psi(\tau_j - \tau^+)\|_2^2 = x + \frac{1}{2} \quad \text{(A3)}$$

with $y_1 + y_2 = 1$. The corresponding jump probabilities read

$$p_1 = \frac{(1 + \mu)y_1}{(1 + \mu)y_1 + (1 - \mu)y_2} \quad \text{(A4)}$$

and

$$p_2 = \frac{(1 - \mu)y_2}{(1 - \mu)y_2 + (1 + \mu)y_1} \quad \text{(A5)}$$

with $p_1 + p_2 = 1$ again. Consequently, a straightforward calculation yields

$$\frac{p_1}{2} - \frac{p_2}{2} = \frac{\mu - 2x}{2 - 4\mu x},$$

(A6)

i.e., the expression in Eq. (12).
the prediction and a comparison for $\Delta = 1$ of the local Lindblad operators and random initial states for the magnetization $\langle S^z_r(t) \rangle$ at the position $r_0 = N/2$ of the local Lindblad operators, as given for weak driving $\mu = 0.1$ by Eq. (11) with amplitudes according to Eq. (12). Curves for various values of the bath coupling $\gamma$ are obtained from the average over 10,000 different trajectories. The other model parameters are the same as in Figs. 2 and 3.

A bath coupling $\gamma/J = 0.1$ is comparable to the jump times in Fig. 2. (a) and (b) correspond to an initial state with and without local magnetization, respectively. In each case, data for $N = 36$ sites is also depicted. (c) Full site dependence for $\gamma/J = 0.1$ in (b).

**Appendix B: Dependence on $\gamma$ and $N$**

Since we have mostly discussed the case of a small bath coupling $\gamma/J = 0.1$, we depict in Fig. 5 the prediction according to Eq. (11) for various values of $\gamma$. We do so for the magnetization $\langle S^z_{r_0}(t) \rangle$ at the position $r_0 = N/2$ of the local Lindblad operators and random initial states $\psi(0)$ with and without local magnetization. Moreover, to demonstrate that this prediction does not depend on system size, we also show the corresponding prediction for $N = 36$ sites.

**Appendix C: Other anisotropies**

In Fig. 4, we have provided a detailed comparison of the dynamics for anisotropy $\Delta = 1.5$, as generated by the full stochastic unraveling procedure and as predicted by Eq. (11). To demonstrate that an agreement of similar quality can be obtained for other anisotropies as well, we show in Fig. 6 a comparison for $\Delta = 1.0$ and $\Delta = 8.0$, as generated by the full stochastic unraveling procedure and as predicted by Eq. (11). Remaining model parameters: Small coupling $\gamma/J = 0.1$, weak driving $\mu = 0.1$, and system size $N = 20$.

**Appendix D: Diffusion coefficient**

Let us, for simplicity, estimate the expansion velocity of the open system by

$$\frac{\nu_{\text{open}}}{D_{\text{closed}}} = \frac{D_{\text{closed}}(t - \bar{\tau})}{D_{\text{closed}}}$$

(D1)

with the average injection time

$$\bar{\tau} = \frac{1}{\gamma} \int_{0^+}^{1} \ln \varepsilon \, d\varepsilon,$$

(D2)

which is $\bar{\tau} J \approx 10$ for $\gamma/J = 0.1$. By taking into account $D_{\text{closed}}/J \approx 0.6$ for $\Delta = 1.5$, one would expect at $t = 2\bar{\tau}$

**FIG. 5.** Time evolution of the magnetization $\langle S^z_r(t) \rangle$ at the position $r_0 = N/2$ of the local Lindblad operators, as given for weak driving $\mu = 0.1$ by Eq. (11) with amplitudes according to Eq. (12). Curves for various values of the bath coupling $\gamma$ are obtained from the average over 10,000 different trajectories. The other model parameters are the same as in Figs. 2 and 3. A bath coupling $\gamma/J = 0.1$ is comparable to the jump times in Fig. 2. (a) and (b) correspond to an initial state with and without local magnetization, respectively. In each case, data for $N = 36$ sites is also depicted. (c) Full site dependence for $\gamma/J = 0.1$ in (b).

**FIG. 6.** Dynamics of the magnetization $\langle S^z_r(t) \rangle$ at various sites $r = r_0 + l$ for anisotropies (a) $\Delta = 1.0$ and (b) $\Delta = 8.0$, as predicted by Eq. (11). Remaining model parameters: Small coupling $\gamma/J = 0.1$, weak driving $\mu = 0.1$, and system size $N = 20$.

**FIG. 7.** Time-dependent spatial variance $\Sigma^2(t)$, as predicted by Eq. (11) for $D_{\text{closed}}/J = 0.6$. 
the expansion velocity
\[ \frac{v_{\text{open}}}{J} \approx \frac{0.6}{2} = 0.3. \] (D3)

Thus, a reasonable expectation is
\[ \Sigma^2(t) = 2v_{\text{open}} t \approx 0.6 tJ. \] (D4)

And indeed, this number is chosen as the prefactor of the power law in Fig. 1.

An alternative and kind of better way to estimate the expansion velocity in the open system is provided by Eq. (11) and the assumption of perfectly diffusive behavior in the closed system (with a zero mean free path). Then, the equilibrium correlation functions take on the simple form
\[ \langle S_r^z(t) S_{r_0}^z(0) \rangle = \frac{1}{4} \exp(-2D_{\text{closed}} t) I_r(2D_{\text{closed}} t), \] (D5)

where \( I_r(t) \) is the modified Bessel function of the first kind and of the order \( r \). By the use of this assumption, the calculation of the time-dependent variance \( \Sigma^2(t) \) in the open system can be done numerically. As depicted in Fig. 7 for \( D_{\text{closed}}/J = 0.6 \), one finds
\[ \Sigma^2(t) \approx 0.66 tJ \] (D6)

over a wide range of time, which is consistent with the simple argument above. Note that the calculation can be easily carried out for \( N = 100 \) of lattice sites.

### Appendix E: Other initial states

The derivation of the prediction in Eq. (11) has relied on an initial pure state \( |\psi(0)\rangle \), which is fully random and corresponds to an equilibrium density matrix at formally infinite temperature. In Fig. 8, we demonstrate that this prediction does not apply to other initial states. To this end, we choose the specific initial pure state
\[ |\psi(0)\rangle \propto (|\uparrow\rangle + |\downarrow\rangle) \otimes \ldots \otimes (|\uparrow\rangle + |\downarrow\rangle), \] (E1)

which is known to be untypical.

![Fig. 8. Analogous comparison as the one in Fig. 4(a), but now the initial pure state |ψ(0)⟩ is not drawn at random.](image-url)
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