

Efficient Computation of Cumulant Evolution and Full Counting Statistics: Application to Infinite Temperature Quantum Spin Chains

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We propose a numerical method to efficiently compute quantum generating functions for a wide class of observables in one-dimensional quantum systems at high temperature. We obtain high-accuracy estimates for the cumulants and reconstruct full counting statistics from the quantum generating functions. We demonstrate its potential on spin $S = 1/2$ anisotropic Heisenberg chain, where we can reach timescales hitherto inaccessible to state-of-the-art classical and quantum simulations. Our results challenge the conjecture of the Kardar-Parisi-Zhang universality for isotropic integrable quantum spin chains.

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Introduction—A complete characterization of the time evolution of a quantum state requires exponential resources as a function of system size and can be carried out only for very small quantum systems [1]. Therefore, one typically follows the strategy of focusing on a specific observable, $\hat{\Sigma}$, often a charge or globally conserved quantity which can fluctuate in a subsystem, and measuring its statistical properties $\Gamma \equiv \Sigma_t - \Sigma_0$ over a time period t . The corresponding distribution $P(\Gamma, t)$ is referred to as the full counting statistics (FCS) [2]. To extract it, one typically performs two measurements, one at a time $t = 0$, to obtain Σ_0 , and another one at time t , to obtain Σ_t .

Only few results are available for the FCS, mainly in quadratic systems [3–9], particular impurity models [10–14], or conformal field theories [15,16] and only recently also in interacting classical [17,18] and quantum [19–22] systems. Experimentally, FCS has been measured in electron transport through tunnel junctions [23–26] and

quantum gases [27]. However, quantum computers and quantum simulators now give direct access to FCS [28–30], as recently demonstrated by the Google Quantum AI experiment [31,32], where the FCS of spin transfer has been analyzed in a discrete space-time analog of the spin $S = 1/2$ anisotropic Heisenberg chain

$$H_{\text{xxz}} = J \sum_{j=1}^{L-1} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right) \quad (1)$$

with S_j^α the α component of the spin $1/2$ operator, J the spin exchange, and Δ the anisotropy parameter.

Recently, it has been conjectured [33,34] that spin transport at the $SU(2)$ -symmetric point of the XXZ model (the Heisenberg limit, $\Delta = 1$) belongs to the Kardar-Parisi-Zhang (KPZ) universality class, which describes space-time correlations in classical interface growth [35,36]. This is striking because integrable spin chains lack key features typical of KPZ physics, such as uncorrelated noise and externally imposed nonequilibrium conditions. The emergence of KPZ scaling in this context has sparked wide interest in the community [27,37–45]. It is now well established that two-point correlation functions in these systems exhibit KPZ scaling with the characteristic superdiffusive exponent $z = 3/2$ [34,45,46]. Remarkably, KPZ behavior has proven to be

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ubiquitous in integrable quantum [43] and classical [47–51] spin chains. Furthermore, KPZ scaling has been identified in both the spin and charge transport channels of the Hubbard model [52], where non-Abelian symmetries and integrability appear crucial for its existence as well. While the microscopic origin remain elusive, it has been suggested that superdiffusion emerges from the hydrodynamics of quasiparticles akin to classical solitons [39,53,54].

Recently, Google’s quantum simulations revealed that, while spin transport is clearly anomalous at the isotropic point, $\Delta = 1$, and consistent with the KPZ scaling of two-point functions [34], the measured skewness and kurtosis of the distribution appear to display a time evolution that is incompatible with those expected for the KPZ universality class [31,32]. To validate the quantum simulations, classical quantum trajectory simulations have been performed, with the initial state sampled using a Monte Carlo method followed by the time evolution of each state. While this approach agreed with the experimental results of Refs. [31,32] within its application range, it is unable to reach substantially longer times.

Here, we propose a quantum generating function (QGF) approach, which is able to reach timescales so far inaccessible to classical quantum trajectory simulations in one-dimensional quantum systems and evaluate cumulant to unprecedentedly long times. We demonstrate the method on a spin $S = 1/2$ anisotropic Heisenberg model [Eq. (1)] at infinite temperature and provide reliable estimates for the FCS and its moments beyond the limits of state-of-the-art experiments.

The quantum generating function approach—Consider a system characterized by a general density operator ρ at time $t = 0$. Performing a projective measurement of $\hat{\Sigma}$ reduces the density matrix to sectors associated with eigenvalues Σ as $\rho \rightarrow \tilde{\rho} = \bigoplus_{\Sigma} \rho_{\Sigma}$, with $\rho_{\Sigma} = P_{\Sigma} \rho P_{\Sigma}$ the projected density operators and P_{Σ} the projector to the subspace of states with eigenvalue Σ . The state described by $\tilde{\rho}$ is then evolved to time t by the time evolution operator $U(t)$, where another projective measurement is performed to extract $\Sigma_t = \Sigma'$. The distribution $P(\Gamma, t)$ is given by

$$P(\Gamma, t) = \sum_{\Sigma, \Sigma'} \delta(\Sigma' - \Sigma - \Gamma) \text{Tr}\{P_{\Sigma'} U(t) \rho_{\Sigma} U^\dagger(t)\}. \quad (2)$$

The quantum trajectory approach samples a state from ρ_{Σ} , performs the time evolution of the state, and measures $\hat{\Sigma}$. The approximation of the distribution $P(\Gamma, t)$ is improved by increasing the number of samples from the initial state. Since the entanglement entropy of a typical initial state rapidly increases, the procedure is computationally expensive. We circumvent this problem by directly computing the generating function of the distribution rather than the distribution itself.

We transform Eq. (2) into a tractable form using the integral representation of the Dirac δ function, $\delta(y) = (1/2\pi) \int_{-\infty}^{\infty} d\lambda e^{i\lambda y}$, and introducing the QGF $G(\lambda, t)$ as

$$G(\lambda, t) \equiv \langle R(\lambda, t) R^\dagger(\lambda, 0) \rangle_{\tilde{\rho}} \quad (3)$$

so that

$$P(\Gamma, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda e^{-i\lambda \Gamma} G(\lambda, t), \quad (4)$$

where the unitary operator $R(\lambda, t) = U(t) e^{i\lambda \hat{\Sigma}} U^\dagger(t) = e^{i\lambda \hat{\Sigma}(t)}$, with $U(t)$ the time-evolution operator and $\langle \cdots \rangle_{\tilde{\rho}} = \text{Tr}[\cdots \tilde{\rho}]$. Two crucial observations are in order here. First, note that $\lim_{\lambda \rightarrow 0} R(\lambda, 0) = \text{id}$, which is a trivial object of vanishing operator entanglement when represented as a matrix product operator (MPO). At small but finite λ the operator $R(\lambda \approx 0, t)$ is, therefore, expected to have limited operator entanglement. The other observation is that, in most cases, the quantity of interest is a sum of commuting *local* observables, $\hat{\Sigma} = \sum_{i \in S} \hat{O}_i$, and, therefore, $R(\lambda, 0) = \bigotimes_{i \in S} e^{i\lambda \hat{O}_i}$, where S defines a subset of sites. In this case, the MPO representation of the operator $R(\lambda, 0)$ is efficient, and operator entanglement is suppressed for small λ . As a result, the computation of $R(\lambda \approx 0, t)$ is relatively inexpensive. Therefore, having an MPO representation of the initial state $\tilde{\rho}$, we can evaluate the trace $\text{Tr}[R(\lambda, t) R^\dagger(\lambda, 0) \tilde{\rho}]$ efficiently (see Fig. 1).

The generating function gives access to the cumulants of the distribution:

$$\kappa_k(t) = (-i)^k \partial_{\lambda}^k \log G(\lambda, t) |_{\lambda=0}. \quad (5)$$

Hence, besides the mean $\mu = \kappa_1$ and variance $\sigma^2 = \kappa_2$, we can characterize the FCS by higher-order (standardized) moments, i.e., skewness $\gamma_3 = \kappa_3/\kappa_2^{3/2}$ and excess kurtosis $\gamma_4 = \kappa_4/\kappa_2^2$ (note that henceforth we drop the explicit time dependence of κ_k and γ_k when convenient). In practice, we evaluate *central moments* [55] from a truncated Taylor expansion of $G(\lambda)$ at a finite value of the counting field $\lambda = |\lambda| e^{i\phi} \in \mathbb{C}$, which we extend to the complex plane:

$$G(\lambda, t) = \sum_{k=0}^{\infty} \frac{1}{k!} |\lambda|^k e^{ik\phi} \mu_k(t). \quad (6)$$

Then μ_k is well approximated by the lowest-order contribution $\propto |\lambda|^{-k}$. With suitable linear combinations of expansions for different phases $\phi = \{0, \pi/2, \pm\pi/4\}$ it is possible to cancel all terms of expansion order

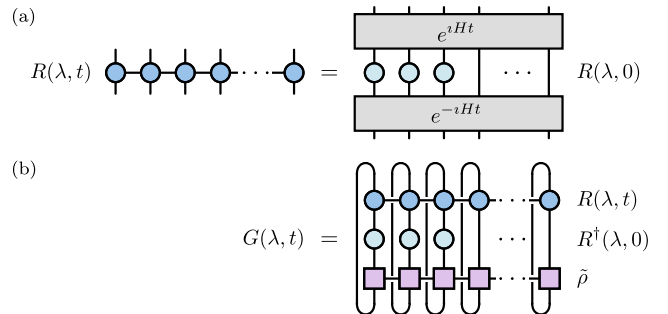


FIG. 1. MPO representation of (a) the unitary operator $R(\lambda, t)$ and (b) the QGF $G(\lambda, t)$.

$m \neq k + 4n$ ($n \in \mathbb{Z}$) and extract moments up to $k \leq 6$ with precision $\mathcal{O}(\lambda^{k+4})$, from which the cumulants can be reconstructed using standard relations (see Supplemental Material [56] for the details). Extracting the cumulants with a high enough precision requires a balance between increasing the maximum MPO bond dimension M , to control the truncation error, and decreasing λ , to control the accuracy of the Taylor expansion. By taking the Fourier transform (4) of $G(\lambda, t)$, we can also reconstruct the distribution $P(\Gamma, t)$.

Infinite temperature anisotropic Heisenberg chain—To demonstrate our method, we analyze spin transfer statistics in the infinite temperature anisotropic Heisenberg chain [Eq. (1)]. We divide the chain into two subsystems, $\mathcal{L}$ and $\mathcal{R}$ of size $L/2$, separated by an interface at bond $j = L/2$, and measure the z component of the spin on the left, $\hat{S} \equiv \sum_{i \in \mathcal{L}} S_i^z$.

We consider an infinite temperature state for which $\tilde{\rho} = \rho \sim \text{id}$, and, therefore, $\tilde{\rho}$ is trivial: $\tilde{\rho} = 2^{-L} \otimes_{j=1}^L \text{id}_j$. We can, therefore, recast the generating function [Eq. (3)] as

$$G_{\text{xxz}}(\lambda, t) = \frac{1}{2^L} \text{Tr}[R(\lambda, t) R^\dagger(\lambda, 0)] \quad (7)$$

with $R(\lambda) = \otimes_{j \in \mathcal{L}} e^{i\lambda S_j^z}$, represented as an MPO. Physically, the operator $R(\lambda)$ generates a twist around the z axis for spins $j \in \mathcal{L}$ by a small angle λ and has a simple form at $t = 0$. The time-evolved operator $R(\lambda, t) = U(t) R(\lambda) U^\dagger(t)$ is obtained numerically by time evolving block decimation (TEBD) [65,66] using the iTensor library [67,68]. The total spin $S_{\text{tot}}^z \equiv \sum_j S_j^z$ commutes with $R(\lambda)$ as well as the time evolution operator $U(t)$ and serves as a U(1) charge in TEBD simulations. To avoid finite size effects, we perform time evolution up to times $tJ < t_{\text{max}}J = L/2$.

Analysis of the spin $S = 1/2$ model—The spin $S = 1/2$ XXZ model is integrable. Spin transport displays *ballistic* and *diffusive* behavior in the easy-plane ($\Delta < 1$) and easy-axis ($\Delta > 1$) regimes, respectively [69]. The two regimes are separated by the isotropic Heisenberg point ($\Delta = 1$) where *superdiffusive* transport emerges [33]. This phenomenology carries over to integrable Trotterized Floquet dynamics [69], studied in Ref. [31]. Figure 2 summarizes our main results; it displays the time evolution of the second cumulant κ_2 and the excess kurtosis, $\gamma_4 = \kappa_4/\kappa_2^2$, obtained by QGF, and compared with other methods as well as with the results of Refs. [31,32].

(a) *The free fermion limit*—On the left-hand side [panels (a) and (d)], we present our results for the XX model at $\Delta = 0$, where transport is ballistic. In this limit, the Hamiltonian (1) can be mapped to noninteracting fermions which allows us to benchmark our numerical simulations against a semianalytical exact solution. Using the Jordan-Wigner transformation [76] and Klich's trace formula [77], Eq. (3) can be cast as the determinant of a matrix whose dimension scales linearly with system size L and is, therefore,

amenable to efficient exact numerical evaluation for large systems (see Supplemental Material [56] for details).

We find perfect agreement between the QGF method and the semianalytical results. This is even more striking when we compare the *local dynamical exponent*, $z^{-1} = (d/d \log t) \log \kappa_2(t)$ [inset in panel (a)]. The second cumulant increases asymptotically in time as $\kappa_2 \propto t^{1/z}$ with $z \rightarrow 1$, in agreement with the prediction of ballistic fluctuation theory (BFT) $\kappa_2 \asymp Jt/(2\pi)$ [56,72]. In Fig. 2, we also present the results of the usual quantum trajectory (QT) approach, which we implemented by exploiting the U(1) symmetry (see Supplemental Material [56] for details). Simulations are performed with a time step $\delta tJ = 1$, favoring faster dynamics to simulate longer timescales while retaining all universal features. The QT approach breaks down at a times $tJ \approx 20$ due to the exploding bond dimensions, while the QGF method provides excellent agreement even for times as large as $tJ \approx 300$.

The excess kurtosis approaches zero as $\gamma_4 \asymp -\pi/(tJ)$, also in excellent agreement with BFT, confirming that at this free fermion point Wick's theorem applies to the joint distribution. This is also supported by investigating the next standardized moment, $\gamma_6 = \kappa_6/\kappa_2^3$ (sextosis; see Supplemental Material [56]). Our semianalytical results show that *all* even cumulants scale linearly in time $\kappa_{2n} \asymp t$, in agreement with the prediction of BFT (see Supplemental Material [56]), implying that the statistics becomes asymptotically Gaussian.

(b) *The isotropic point*—The central panels in Fig. 2 focus on the isotropic point, $\Delta = 1$, where a direct comparison with experiments is also possible. The isotropic point is of particular interest, as we can investigate whether the scaling of higher-order cumulants supports the KPZ conjecture for isotropic integrable quantum spin chains [34].

The QGF method confirms superdiffusive dynamics at the isotropic point with the KPZ exponent $\kappa_2 \propto t^{2/3}$, $z \rightarrow 3/2$, both for time steps $\delta tJ = 1$ and for $\delta tJ = 4\pi/5 \approx 2.51(3)$ [78], corresponding to the fSim gates used in the Google experiments (see the derivation in Supplemental Material) [31]. Remarkably, the QGF method remains stable for times far beyond the quantum simulations of Ref. [31] as well as QT simulation times; it agrees with the experiments and QT at times $tJ \lesssim 20$ but clearly signals the breakdown of both at times $tJ \approx 20$.

In contrast to κ_2 , the kurtosis γ_4 presented in Fig. 2(e) is, however, clearly inconsistent with KPZ scaling [31]. Although experimental values of $\gamma_4(t)$ become unreliable at times $tJ \gtrsim 20$, a jackknife estimate provides an asymptotic value $\gamma_4^{\text{jackknife}} = -0.05 \pm 0.02$ [31], which is incompatible with the kurtosis from Baik-Rains [73] and Tracy-Widom [74] distributions, characterizing phenomena in the KPZ universality class [79].

Our QGF simulations confirm the overall conclusions of Ref. [31] but provide a refined picture over significantly

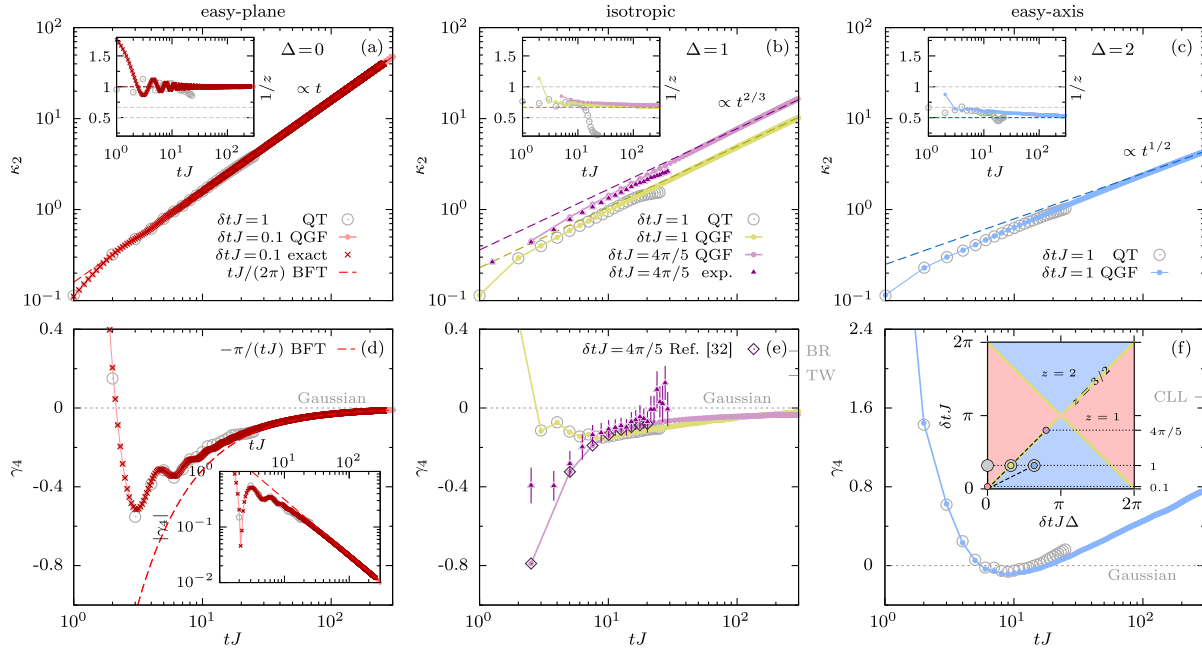


FIG. 2. Time evolution of the variance κ_2 with the corresponding dynamical exponent z [panels (a)–(c) and insets] and of the excess kurtosis $\gamma_4 = \kappa_4/\kappa_2^2$ [panels (d)–(f)] in the easy-plane ($\Delta = 0$), isotropic ($\Delta = 1$), and easy-axis ($\Delta = 2$) regimes. In the XX limit (a), (d), QGF quasicontinuous time evolution ($\delta tJ = 0.1$) is validated against exact numerical results and predictions of asymptotic behavior from BFT [70–72]. At the isotropic point (b), (e), the Floquet evolution ($\delta tJ = 1$) is compared against recent experimental data [31,32]. To compensate for different charge conventions, the κ_2 data from Ref. [32] have to be rescaled by a factor $r_2 = 32$, whereas rescaling factors cancel out in the kurtosis. The time step $\delta tJ = 4\pi/5$ is chosen to match that of the experimental fSim gates. The simulation for γ_4 perfectly reproduce the exact density matrix simulations from Ref. [32]. Predictions for the asymptotic kurtosis γ_4 confirm the experimental conclusions and are inconsistent with values from the Baik-Rains (BR) [73] and Tracy-Widom (TW) [74] distributions, expected in the KPZ universality class, depending on the initial condition. In the easy-axis regime (c), (f), the statistics is strongly non-Gaussian, and, despite the slow convergence, the kurtosis is compatible with the estimate from the classical Landau-Lifshitz magnet (CLL) [75]. In all regimes, the QT simulations are performed with a time step $\delta tJ = 1$. The schematic phases diagram [inset in panel (f)] identifies the ballistic ($z = 1$, red), superdiffusive ($z = 3/2$, yellow), and diffusive ($z = 2$, cyan) transport regimes, whereas the symbols correspond to the QGF and QT simulations in the phase diagram. Parameters: $M = 2^6$ ($\Delta = 0$) and $M = 2^{10}$ ($\Delta \neq 0$), $\lambda = 0.03$, and different δtJ (as labeled).

longer times. The QGF γ_4 data agree perfectly with experimental results over the first few cycles and with density matrix simulations in Refs. [31,32]. However, Floquet time evolution [69] (performed with $\delta tJ = 1$ and $\delta tJ = 4\pi/5$) yield a time evolution consistent both with asymptotic Gaussian fluctuations, $\gamma_4 \rightarrow 0$, or weakly non-Gaussian fluctuations with slightly negative kurtosis, $\gamma_4 < 0$. Similarly, the next nonzero standardized moment $\gamma_6 = \kappa_6/\kappa_2^3$ falls rapidly with time. Within the accuracy of the simulation, it remains difficult to discriminate between asymptotic Gaussian fluctuations, $\gamma_6 \rightarrow 0$, or weakly non-Gaussian fluctuations with slightly positive sextosis, $\gamma_6 > 0$ (see Supplemental Material [56]).

(c) *Easy-axis regime*—We now focus on the easy-axis regime, where we present simulations for $\Delta = 2$ in the right panels in Fig. 2. Here, $\kappa_2 \propto t^{1/2}$ reveals diffusive behavior with $z \rightarrow 2$, but the numerics suggests an asymptotic kurtosis $\gamma_4 > 0$, corresponding to a strongly non-Gaussian distribution. The kurtosis data do not show any clear sign of saturation in the investigated time window. This

is not surprising, since even the dynamical exponent converges rather slowly toward $z = 2$; see the inset in Fig. 2(c). A similarly slow convergence has been observed in a related model, the classical Landau-Lifshitz magnet, with asymptotic kurtosis $\gamma_4^{\text{CLL}} = 3(\pi/2 - 1)$ [75], indicated for reference in Fig. 2(f) and still compatible with our numerics.

Scaling properties of the generating function and full counting statistics—Our method allows one to extract the generating function $G(\lambda, t)$ as a function of λ and t , to reconstruct $P(\Gamma, t)$ by performing the Fourier transformation (4). In Fig. 3, we present results for the isotropic point, $\Delta = 1$ (the ballistic and diffusive regimes are discussed in Supplemental Material [56]). The curves in Fig. 3(a) correspond to snapshots of $G(\lambda, t)$ at different times. Upon rescaling the counting field as $\lambda \rightarrow \lambda t^{1/2z}$, the data collapse to a single curve, as shown in the inset for the QT and QGF methods. Analogously, Fig. 3(b) demonstrates the collapse of the rescaled distributions $P(\Gamma, t) \rightarrow \mathcal{P}_{1/2z}(\Gamma/t^{1/2z}) = t^{1/2z}P(\Gamma/t^{1/2z}, t)$. In both cases, the data collapse is obtained using the appropriate

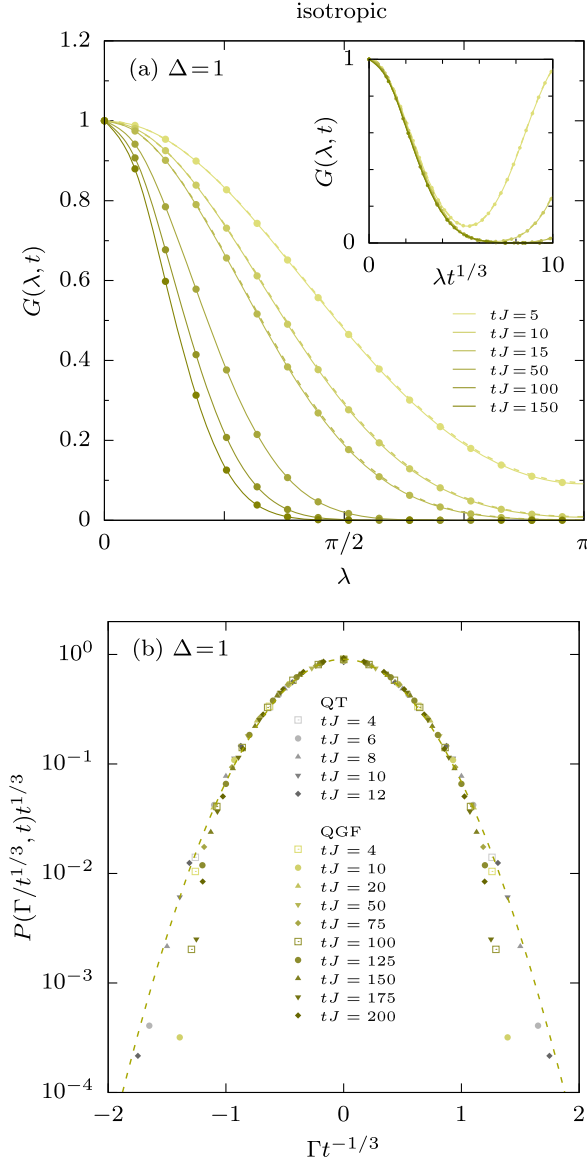


FIG. 3. (a) Generating function at different time snapshots obtained with QT (dashed) and QGF (solid lines) and their scaling collapse (insets) at the isotropic Heisenberg point ($\Delta = 1$). (b) Scaling collapse of FCS for QT (gray gradient symbols) and QGF (color gradient symbols). The rescaled distribution $\mathcal{P}_{1/3}(\Gamma/t^{1/3}) \equiv t^{1/3}P(\Gamma/t^{1/3}, t)$ becomes a function of $\Gamma/t^{1/3}$, corresponding to a dynamical exponent, $z = 3/2$. Dashed lines represent a Gaussian distribution, for comparison. Parameters: $M = 2^{10}$ and $\delta tJ = 1$.

dynamical exponent $z = 3/2$ for $\Delta = 1$. Although the data are not entirely decisive, at the isotropic (Heisenberg) point, the tails of the distribution appear thinner than Gaussian, in qualitative agreement with the evolution of the kurtosis [see Fig. 2(e)], which is calculated with higher accuracy, and represents the main evidence for non-Gaussianity.

Conclusions and outlook—We introduced a quantum generating function approach to accurately and efficiently compute the full counting statistics for sums of local

observables and their corresponding moments. We demonstrated this method on the anisotropic spin $S = 1/2$ XXZ model. Benchmarking for $\Delta = 0$ against numerically exact solutions confirmed the astonishing accuracy and range of validity of the QGF method. We are able to extract even time derivatives with high accuracy and over timescales more than an order of magnitude beyond those of quantum simulations in Ref. [31] as well as quantum trajectory approaches. At the isotropic point, $\Delta = 1$, our results are consistent with a vanishing or a weakly negative kurtosis, demonstrating that spin transfer statistics is inconsistent with KPZ scaling. Our method is widely applicable to one-dimensional systems with U(1) conserved charges, in arbitrary initial states. In particular, we recently applied it to demonstrate the emergence of self-similar Family-Vicsek scaling in integrable and nonintegrable quantum SU(N) spin chains [80].

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