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Spin diffusion in the one-dimensional $s = \frac{1}{2} XXZ$ model at infinite temperature

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Time-dependent spin-autocorrelation functions at $T = \infty$ and (in particular) their spectral densities for the bulk spin and the boundary spin of the semi-infinite spin- $\frac{1}{2} XXZ$ model (with exchange parameters $J_x = J_y \equiv J, J_z$) are investigated on the basis of (i) rigorous bounds in the time domain and (ii) a continued-fraction analysis in the frequency domain. We have found strong numerical evidence for spin diffusion in quantum spin models. For J_z/J increasing from zero, the results of the short-time expansion indicate a change of the bulk-spin xx-autocorrelation function from Gaussian decay to exponential decay. The continued-fraction analysis of the same dynamic quantity signals a change from exponential decay to power-law decay as J_z/J approaches unity and back to a more rapid decay upon further increase of that parameter. By contrast, the change in symmetry at $J_z/J = 1$ has virtually no impact on the bulk-spin zz-autocorrelation function (as expected). Similar contrasting properties are observable in the boundary-spin autocorrelation functions.

I. INTRODUCTION

After more than two decades of theoretical studies devoted to high-temperature dynamics of quantum spin chains, which have produced a number of intriguing exact results, one central question has remained unanswered: Does the phenomenological concept of spin diffusion provide at all an adequate description for the transport of the fluctuations of a conserved magnetization component? While the spin-diffusion phenomenon was frequently invoked for the interpretation of experimental results from inelastic neutron scattering, electron spin resonance and NMR on quasi-one-dimensional (1D) magnetic compounds,^{1,2} its support by microscopic theories or numerical analysis of quantum spin dynamics has remained rather weak and tentative³⁻⁵ or artificially imposed.⁶

Even for *classical* spin chains, whose long-time dynamics is more readily accessible to numerical analysis by means of simulation studies, the answer to that question has proven to involve unanticipated subtleties. The anomalous character of spin diffusion in the classical Heisenberg chain, identified some five years ago,⁷ has remained a matter of controversy ever since as to its correct interpretation.⁸⁻¹³ There is now strong evidence that the diffusivity is singular, giving rise to logarithmic corrections in the long-time tail of the spinautocorrelation function,¹² but the exact nature of these corrections and their origin have remained obscure.

It is much more challenging to analyze the long-time dynamics of *quantum* spin chains. There are only very few quantum spin models with nontrivial dynamics for which dynamic correlation functions at $T = \infty$ have been determined exactly. Among them are the equivalent-neighbor XXZ model^{14,15} and the 1D $s = \frac{1}{2}XY$ model.¹⁶⁻²³ Spin diffusion has no part in either model for

reasons that are well understood.

For other quantum spin models with nontrivial dynamics, such as the 1D XXZ model, exact information on dynamic correlation functions is limited to a number of frequency moments obtained from $T = \infty$ expectation values of spin products.^{5,24-26} The information contained in these frequency moments can be employed in two different ways to infer characteristic properties of dynamic correlation functions:

(i) We may use the frequency moments as Taylor coefficients in the short-time expansion of a correlation function. For certain situations, the rigorous upper and lower bounds thus determined for that function may yield accurate results over time intervals that are sufficiently long to unlock valuable information on the underlying physical process—information that is otherwise inaccessible.

(ii) For certain other situations, further information on the long-time behavior can be extracted from the frequency moments if they are converted into an equal number of continued-fraction coefficients for the relaxation function (the Laplace transform of the correlation function).

This paper builds principally on the accomplishments of two previous studies of $T = \infty$ quantum spin dynamics^{23,25} with focus on methods (i) and (ii), respectively. Here the analytic and numerical techniques developed in those studies are combined for the specific purpose of elucidating the $T = \infty$ dynamics of the 1D $s = \frac{1}{2} XXZ$ model. The Hamiltonian for a semi-infinite chain reads

$$H_{XXZ} = -\sum_{l=0}^{\infty} \left\{ J(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + J_z S_l^z S_{l+1}^z \right\} .$$
(1.1)

We focus on (normalized) spin-autocorrelation functions

$$C^{\mu\mu}(t) \equiv \frac{\langle S^{\mu}_{l}(t)S^{\mu}_{l} \rangle}{\langle S^{\mu}_{l}S^{\mu}_{l} \rangle}, \quad \mu = x, z$$
(1.2)

at $T = \infty$ and the associated spectral densities

$$\Phi_l^{\mu\mu}(\omega) \equiv \int_{-\infty}^{+\infty} dt \ e^{i\omega t} C_l^{\mu\mu}(t), \quad \mu = x, z \ . \tag{1.3}$$

Results will be presented for $l = \infty$ (bulk spin) and l=0 (boundary spin). For two special cases, the dynamics can be analyzed exactly: the XX model $(J_z=0)$ is equivalent to a system of noninteracting lattice fermions, and the X model (J=0) is as trivial as the quantum harmonic oscillator. For other parameter values, however, the $T = \infty$ dynamics of the XXZ model is quite complicated, and transitions between different types of dynamical behavior can be studied. For that purpose, the two above-mentioned methods (i) and (ii) of analyzing frequency moments turn out to be invaluable instruments for analysis and interpretation. Our main point of emphasis is the identification of diffusive long-time tails in spin-autocorrelation functions under the right symmetry conditions or the corresponding infrared divergences in the associated spectral densities.

The phenomenon of spin diffusion is based on a thermalization process that is subject to a conservation law. The phenomenological theory in its simplest form states that the fluctuations $S^{\mu}(q,t)$ of any conserved spin component satisfy the diffusion equation for sufficiently long times and wavelengths. It predicts exponential decay for correlation functions that are not constrained by that conservation law and diffusive long-time tails for those that are. The fact is that exponential decay in time or diffusive long-time tails do not occur in any of the

known exact results for interacting quantum spin systems. The decay in those systems turns out to be either Gaussian or nondiffusive power law. In this study we provide evidence in support of spin diffusion in the 1D $s = \frac{1}{2} XXZ$ model in the form of a crossover from Gaussian to exponential decay (Sec. III) and in the form of long-time tails that come and go with the conservation law required for diffusive behavior (Secs. IV-VI). The presentation of the results is preceded (Sec. II) by a brief description of the two main methods of analysis employed here.

II. CALCULATIONAL TECHNIQUES

At $T = \infty$, the spin-autocorrelation function (1.2) is real and symmetric. It can be expanded into a power series of the form

$$C_{l}^{\mu\mu}(t) = \sum_{k=0}^{\infty} \frac{(-1)^{k}}{(2k)!} M_{2k}^{\mu\mu}(l) t^{2k} , \qquad (2.1)$$

where the expansion coefficients are the frequency moments of the spectral density (1.3)

$$M_{2k}^{\mu\mu}(l) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega^{2k} \Phi_l^{\mu\mu}(\omega)$$

= $(-1)^k \left[\frac{d^{2k}}{dt^{2k}} C_l^{\mu\mu}(t) \right]_{t=0}, \quad k = 0, 1, 2, \dots, \quad (2.2)$

and can be expressed as expectation values

$$M_{2k}^{\mu\mu}(l) = -(-1)^{l} \langle [\cdots [S_{l}^{\mu}, H], \dots, H] [\cdots [S_{l}^{\mu}, H], \dots, H] \rangle / \langle S_{l}^{\mu} S_{l}^{\mu} \rangle$$

$$(2.3)$$

of operators produced by the product of two k-fold commutators.^{5,25} These expectation values can be evaluated exactly by readily programmable integer arithmetic as explained in Ref. 25. We have determined the $M_{2k}^{\mu\mu}(l)$ up to k = 14 for the bulk spin $(l = \infty)$ of the XXZ model and up to k = 17 for the boundary spin (l = 0). This represents a significant advance from previously known moments for that model.^{5,24} The exact moments are listed in Appendix A.

In Sec. III we shall use these expansion coefficients to determine upper and lower bounds of the spinautocorrelation function by methods that have been developed and described previously.^{5,24-27} In Secs. IV-VI the information contained in the frequency moments will be analyzed by quite different methods. We convert the $M_{2k}^{\mu\mu}(l)$ into the continued-fraction coefficients $\Delta_{k}^{\mu\mu}(l)$ of the relaxation function

$$c_{l}^{\mu\mu}(z) \equiv \int_{0}^{\infty} dt \ e^{-zt} C_{l}^{\mu\mu}(t) = \frac{1}{z + \frac{\Delta_{1}^{\mu\mu}(l)}{z + \frac{\Delta_{2}^{\mu\mu}(l)}{z + \cdots}}}, \qquad (2.4)$$

which is the Laplace transform of the spinautocorrelation function (1.2), and proceed with the analysis from there. A set of transformation formulas between the first K frequency moments $M_{2k}^{\mu\mu}(l)$ and the first K coefficients $\Delta_k^{\mu\mu}(l)$ is given in Appendix B.

It must be mentioned that the continued-fraction coefficients $\Delta_k^{\mu\mu}(l)$ can be determined more directly by means of the recursion method. The computational effort is almost identical to that required for the determination of an equal number of frequency moments $M_{2k}^{\mu\mu}(l)$. A brief account of Lee's²⁸ formulation of the recursion method as applied to quantum spin dynamics at high temperature was given in Refs. 15, 21, and 23 for several applications.

In this paper, the known continued-fraction coefficients $\Delta_k^{\mu\mu}(l)$ will be analyzed along two different lines: (a) We shall reconstruct the spectral density (1.3) from the relaxation function (2.4) via the relation

$$\Phi_l^{\mu\mu}(\omega) = 2 \lim_{\varepsilon \to 0} \mathcal{R}[c_l^{\mu\mu}(\varepsilon - i\omega)]$$
(2.5)

by methods involving the use of matching termination functions that have previously been tested and applied in quantum spin dynamics.^{23,29,30} (b) We shall employ the method developed in Ref. 30 for the identification of infrared singularities in spectral densities by direct analysis of the known sequence of $\Delta_k^{\mu\mu}(l)$.

III. FROM GAUSSIAN DECAY TO EXPONENTIAL RELAXATION

Consider first the bulk-spin autocorrelation function $\langle S_{\infty}^{x}(t)S_{\infty}^{x} \rangle$ of the XXZ model (1.1). The nontrivial but exactly solvable case $J_{z} = 0$ (XX model) is an ideal starting point for the analysis of the XXZ cases by both calculational techniques we intend to employ. The well-known exact expressions for that autocorrelation function and its spectral density in the XX limit read:¹⁸⁻²¹

$$\left\langle S_{\infty}^{x}(t)S_{\infty}^{x}\right\rangle = \left\langle S_{\infty}^{y}(t)S_{\infty}^{y}\right\rangle = \frac{1}{4}e^{-J^{2}t^{2}/4}, \qquad (3.1)$$

$$\Phi_{\infty}^{xx}(\omega) = \frac{2\sqrt{\pi}}{J} e^{-\omega^2/J^2} . \qquad (3.2)$$

The Gaussian decay of (3.1) is clearly anomalous, attributable to the free-fermion nature of the XX model. The default expectation within the spin-diffusion scenario would be exponential decay at long times instead. The nongeneric processes that govern the transport of spin fluctuations in the XX model are further indicated by the fact that all pair-correlation functions $\langle S_l^x(t)S_{l'}^x\rangle$, $l\neq l'$ are identically zero. In the XXZ model, the anomalous features are expected to disappear. A weak fermion interaction (with coupling constant J_z) impacts the longtime behavior more strongly than it affects the short-time behavior. In the function $\langle S_{\infty}^{x}(t)S_{\infty}^{x} \rangle$ we thus expect to see a crossover from a Gaussian behavior at short times to exponential decay at longer times. The very simple structure of the exact result (3.1) makes it possible to observe clear indicators for such a crossover in a short-time expansion at $J_z \ll J$.

In Fig. 1 we have plotted the function $\ln(\langle S_{\infty}^{x}(t)S_{\infty}^{x}\rangle)/(Jt\langle S_{\infty}^{x}S_{\infty}^{x}\rangle)$ versus Jt for four

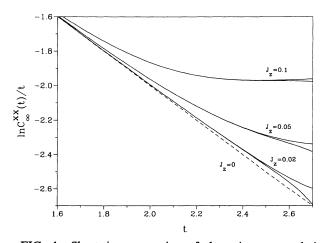


FIG. 1. Short-time expansion of the spin-autocorrelation function $C_{\infty}^{xx}(t) = \langle S_{\infty}^{x}(t) S_{\infty}^{x} \rangle / \langle S_{\infty}^{x} S_{\infty}^{x} \rangle$ at $T = \infty$ of the 1D $s = \frac{1}{2}$ XXZ model for J = 1 and $J_z = 0.02$, 0.05, 0.1 (solid lines) near the exactly solvable case $J_z = 0$ (dashed line). The data are plotted in a way suitable for visualizing the crossover from Gaussian decay (negative unit slope) to exponential decay (zero slope). Each result of the short-time expansion is represented by two curves corresponding to an upper and a lower bound of the function. The bounds have been determined from 14 exact frequency moments $M_{2k}^{xx}(\infty)$.

different parameter values of the XXZ model near the XX limit. The straight dashed line with negative slope represents the pure Gaussian (3.1). The results for $J_z \neq 0$ show strong indications that the decay is slower than Gaussian, consistent with exponential decay (convergence toward a negative constant in the plot of Fig. 1). Powerlaw decay would imply convergence toward zero. Whether or not the observed exponential decay represents the true asymptotic behavior is, of course, beyond the reach of this type of analysis.

IV. FROM EXPONENTIAL RELAXATION TO DIFFUSIVE LONG-TIME TAILS

Unlike in classical spin dynamics, where diffusive long-time tails are readily detectable in simulation data and directly amenable to a quantitative analysis, the most direct indicators of their presence in quantum spin dynamics (at least in 1D and 2D systems) are infrared divergences in spectral densities. The continued-fraction analysis is an ideal instrument for the quantitative study of such singularities.

A. Δ_k sequences and model spectral densities

The exact result (3.2) for the spectral density $\Phi_{\infty}^{xx}(\omega)$ of the XX model can be reproduced by means of the recursion method with relative ease. It is determined by the linear sequence

$$\Delta_k^{xx}(\infty) = \frac{1}{2}J^2k \quad (J_z = 0) \tag{4.1}$$

via (2.4) and (2.5).²¹ The strength of the continuedfraction analysis of this function derives from the fact that gradual deviations from the exactly solvable limit $J_z = 0$ produce only gradual deviations from (4.1). The resulting nearly linear Δ_k sequences, in turn, produce gradual changes in the spectral density $\Phi_{\infty}^{xx}(\omega)$.

As J_z increases from zero, we can identify two types of systematic deviations of the Δ_k 's from the linear sequence (4.1): (i) A gradual increase in growth rate λ implies a gradual change in the decay law at large ω of the spectral density according to the following relation:^{31,32}

$$\Delta_k^{\mu\mu}(l) \sim k^{\lambda} \Longleftrightarrow \Phi_l^{\mu\mu}(\omega) \sim \exp(-|\omega|^{2/\lambda}) . \tag{4.2}$$

(ii) Gradually increasing alternating deviations of the Δ_k 's from the line k^{λ} signal the emergence of a powerlaw singularity at $\omega = 0$ in the spectral density and allow for an estimate of the singularity exponent.^{23,30} Both effects are illustrated in Fig. 2. The main plot shows $\ln \Delta_k$ versus $\ln k$ for two cases of the XXZ model. The open circles represent the linear sequence (4.1) for $J_z = 0$, which has slope $\lambda = 1$. The regression line for $J_z = J$ has slope $\lambda \simeq 1.22$. The predominantly alternating deviations of the full circles from that line are clearly visible. The inset shows the variation of the growth rate λ with J_z between the XX and XXX models.³³ Changes in growth rate over that range have only negligible impact on the physically interesting structures in the spectral densities investigated here. The growing alternating deviations in the Δ_k sequence are the signature of an emerging infrared divergence implied by the spin-diffusive long-time tail that is

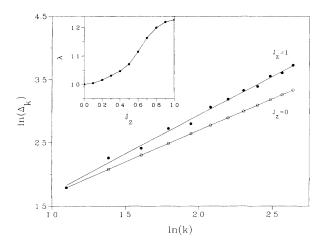


FIG. 2. Log-log plot of the sequences $\Delta_k^{xx}(\infty)$ for the bulkspin-autocorrelation function $\langle S_{\infty}^x(t)S_{\infty}^x \rangle$ at $T = \infty$ of the 1D $s = \frac{1}{2} XX \mod (J = 1, J_z = 0)$ and XXX model $(J = J_z = 1)$. The slope of the linear regression lines determines the growth rate λ of each Δ_k sequence. The inset shows λ as a function of J_z (for J = 1).

expected to dominate the function $\langle S_{\infty}^{x}(t)S_{\infty}^{x} \rangle$ for $J_{z}=J$. A quantitative analysis of that singularity will be presented in Sec. IV C. It yields strong evidence for a transition from an unconstrained relaxation process at $J_{z} < J$ to a diffusion process at $J_{z}=J$ in the fluctuations of $S_{\infty}^{x}(t)$.

For the reconstruction of spectral densities from Δ_k sequences with growth rates $\lambda \simeq 1$, we have proposed and successfully employed the following procedure:^{29,30} Pick a Gaussian model spectral density, (i) $\overline{\Phi}(\omega) = (2\sqrt{\pi}/\omega_0) \exp(-\omega^2/\omega_0^2)$. (ii) Expand the associated model relaxation function (2.4) into a continued fraction down to level n; this generates the model coefficients $\overline{\Delta}_k = \omega_0^2 k/2$ and defines the *n*th-level termination function $\Gamma_n(z)$. (iii) Determine the parameter ω_0 by matching the slope of $\overline{\Delta}_k$ versus k with the average slope of $\Delta_k^{xx}(\infty)$ vs k for the finite sequence of coefficients $\Delta_1^{xx}(\infty), \ldots, \Delta_n^{xx}(\infty)$ pertaining to the dynamical quantity of interest and inferred from exact moments or produced by the recursion method. (iv) Replace the model coefficients $\overline{\Delta}_1, \ldots, \overline{\Delta}_n$ by the known system coefficients $\Delta_1^{xx}(\infty), \ldots, \Delta_n^{xx}(\infty)$ in the relaxation function and evaluate the spectral density via (2.5). That is the recipe for reconstructing spectral densities by means of a Gaussian terminator.

For Δ_k sequences whose growth rates deviate significantly from $\lambda = 1$ and whose spectral densities are likely to have infrared divergences as their dominant structure we should carry out such an analysis on the basis of the more general model spectral density

$$\overline{\Phi}(\omega) = \frac{2\pi/\lambda\omega_0}{\Gamma\left[\frac{\lambda}{2}(1+\alpha)\right]} \left|\frac{\omega}{\omega_0}\right|^{\alpha} \exp(-|\omega/\omega_0|^{2/\lambda}). \quad (4.3)$$

This remains impractical as long as we lack closed-form expressions for the model continued-fraction coefficients Δ_k pertaining to (4.3) as functions of the three parame-

ters $\omega_0, \alpha, \lambda$. However, for growth rates sufficiently close to $\lambda = 1$, we can approximate the $(\lambda \neq 1)$ problem with a $(\lambda = 1)$ problem if we replace the Δ_k sequence by the rescaled sequence

$$\Delta_k^* = \Delta_k^{1/\lambda} \tag{4.4}$$

and then proceed as outlined previously. The main distortions in the reconstructed spectral density caused by this approximation are of two kinds: (i) a change in the large- ω decay law and (ii) a change in the frequency scale. Whereas the former effect has only a negligible impact on the shape of the spectral-weight distribution, the latter may warrant attention and lead to significant improvement upon proper adjustment.³⁴

B. Reconstruction of spectral densities

We have reconstructed the bulk-spin spectral density $\Phi_{\infty}^{xx}(\omega)$ of the XXZ model for $0 \le J_z/J \le 1$ by using the continued-fraction coefficients $\Delta_1^{xx}(\infty), \ldots, \Delta_{14}^{xx}(\infty)$ inferred from the moments tabulated in Appendix A and a Gaussian terminator with its parameter determined from the slope of the Δ_k^* sequence.

Figure 3 shows the reconstructed function $\Phi_{\infty}^{xx}(\omega)$, at $\omega < 0$ for values of the anisotropy parameter between $J_z/J = 0$ and $J_z/J = 0.5$, and at $\omega > 0$ for parameter values between $J_z/J = 0.6$ and $J_z/J = 1.0$. The five curves on the left illustrate how the pure Gaussian (3.2) (dashed line) evolves into a curve with some structure as J_z/J increases from zero. The additional structure consists of (i) a central peak of increasing height and decreasing width and (ii) a shoulder of enhanced spectral weight

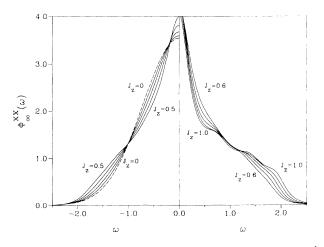


FIG. 3. Spectral density $\Phi_{\infty}^{xx}(\omega)$ at $T = \infty$ of the 1D $s = \frac{1}{2}$ XXZ model with J = 1 as reconstructed from the continuedfraction coefficients $\Delta_1^{xx}(\infty), \ldots, \Delta_{14}^{xx}(\infty)$ and a Gaussian terminator. The calculation was carried out by the use of the Δ_k^* sequence in the role of the original Δ_k sequence. The four solid curves for $\omega < 0$ pertain to the values $J_z = 0.2, \ldots, 0.5$ of the anisotropy parameter and the five curves plotted for $\omega > 0$ to values $0.6, \ldots, 1.0$. The dashed curve represents the exact result (3.2) for the case $J_z = 0$. The result for $J_z = 0.1$ (not shown) deviates from that for $J_z = 0$ by amounts comparable to the thickness of the dashed line.

at $\omega \simeq 1.5J$. The further development of the spectral density as J_z/J approaches the XXX case is shown by the curves on the right. The shoulder becomes more pronounced, and the strong peak at $\omega = 0$, signals the presence of an infrared divergence for $J_z = J$ in accordance with spin-diffusion phenomenology.

The curve for the XXX case is in qualitative agreement with previous results obtained from finite-chain calculations,^{3,4} and by a calculation which uses the first two frequency moments of the dynamic structure factor in conjunction with a two-parameter diffusivity.⁶ We should like to emphasize that the infrared singularity in $\Phi_{\infty}^{xx}(\omega)$, which is strongly suggested by the curves for $J_z/J \simeq 1$ in Fig. 3, is in no way artificially built into our approach. It is a structure resulting solely from the 14 known continued-fraction coefficients.

The reconstructed spectral density $\Phi_{\infty}^{xx}(\omega)$ shown in Fig. 3 is expected to be most accurate for small values of J_z/J , where the growth rate is closest to $\lambda = 1$ (see Fig. 2, inset). As the growth rate increases toward $\lambda \simeq 1.22$, the curves are likely to become subject to the above-mentioned systematic errors. We have estimated the systematic error in frequency scale not to exceed 2% for the curves at $0 < J_z/J \le 0.5$ and 12% for those at $0.5 < J_z/J \le 1$.

C. Analysis of infrared singularities

For a quantitative analysis of the infrared singularity in the spectral density $\Phi_{\infty}^{xx}(\omega)$, we focus on the alternating deviations about the average (nearly linear) growth of the Δ_k sequences. Consider the special case $\lambda=1$ of the model spectral density (4.3). The associated Δ_k sequence is known in closed form:²⁹

$$\overline{\Delta}_{2k-1} = \frac{1}{2}\omega_0^2(2k-1+\alpha), \quad \overline{\Delta}_{2k} = \frac{1}{2}\omega_0^2(2k) \ . \tag{4.5}$$

For this model spectral density, the singularity exponent α is determined by the displacement of the $\overline{\Delta}_{2k-1}$ from the line $\overline{\Delta}_{2k} = \omega_0^2 k$. In real situations, that displacement is subject to "fluctuations" caused by other structures in the spectral density. The exponent α of the infrared singularity can nevertheless be estimated from the average distance in vertical displacement of the Δ_{2k} and the Δ_{2k-1} from the linear regression line for the entire sequence. Two previous applications of that procedure yielded reasonable results.^{23,30}

The results of such an analysis applied to the Δ_k^* sequences inferred from 14 exact moments are compiled in Fig. 4. The full circles joined by solid lines represent the mean exponent values α as a function of J_z/J ranging from the XX model ($J_z=0$) to the XXX model ($J_z=J$) and somewhat beyond. The error bars indicate the statistical uncertainty for each data point, which is due to the fact that the analysis is based on a finite number of known continued-fraction coefficients. On top of the statistical error, the data are likely to be subject to a systematic error whose potential impact increases with the deviation of the growth rate from $\lambda=1$. We have yet to design a simple and satisfactory way to correct for systematic errors in the exponent analysis. As J_z ap-

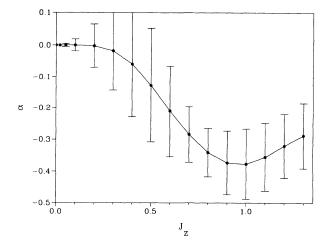


FIG. 4. Infrared-singularity exponent α versus anisotropy parameter J_z of the spectral density $\Phi_{\infty}^{xx}(\omega)$ at $T = \infty$ of the 1D $s = \frac{1}{2}$ XXZ model with J = 1. The data points were obtained from the continued-fraction coefficients $\Delta_3^{xx}(\infty), \ldots, \Delta_{14}^{xx}(\infty)$ by analyzing the associated Δ_k^* sequence.

proaches zero, both types of uncertainties (statistical and systematic) become smaller and disappear. The data point $\alpha(0)=0$ is exact and describes the spectral density (3.2), which has no infrared singularity.

In spite of the limited overall accuracy of these results, the dependence on J_z/J of the mean exponent values displayed in Fig. 4 is quite remarkable. The data strongly indicate that the function $\alpha(J_z/J)$ stays zero over some range of the anisotropy parameter. A vanishing exponent at small but nonzero J_z/J is consistent with and thus reinforces the conclusion reached from the short-time analysis that the function $\langle S_{\infty}^x(t) S_{\infty}^x \rangle$ decays faster than a power law.

While the data point at $J_z/J=0.5$ is still consistent with $\alpha=0$, the mean α values have already a strongly decreasing trend at this point. A minimum value is reached exactly at the symmetry point $(J_z=J)$ of the XXX model—the only point for which the conservation law $S_T^x = \sum_i S_i^x = \text{const}$ holds, and therefore the only point for which one expects a diffusive long-time tail in $\langle S_{\infty}^x(t)S_{\infty}^x \rangle$. Upon further increase of J_z/J , the data points rise again toward $\alpha=0$ as expected.

The minimum exponent value, $\alpha = -0.37 \pm 0.12$, obtained for the XXX case is only marginally consistent with the standard value, $\alpha = -\frac{1}{2}$, predicted by spindiffusion phenomenology. That discrepancy is more likely attributable to the systematic error in our data than it is evidence for anomalous spin diffusion such as was discovered in the classical 1D XXX model.⁷⁻¹³

V. SUSTAINED POWER-LAW DECAY

The conservation law $S_T^z = \sum_i S_i^z = \text{const}$ for the spin fluctuations in the z direction holds over the entire parameter range of the XXZ model. Consequently, the long-time behavior of the correlation function $\langle S_{\infty}^z(t) S_{\infty}^z \rangle$ or the low-frequency behavior of the spectral density $\Phi_{\infty}^{zz}(\omega)$ is expected to be much less affected by

for quantum spin diffusion. Here the kind of analysis carried out previously for the reconstruction of spectral densities (Sec. IV B) and for the estimation of singularity exponents (Sec. IV C) becomes inapplicable for $0 \le J_z/J \le 0.6$. The breakdown is caused by a crossover in the growth rates of the relevant sequences of continued-fraction coefficients. Figure 5 shows the Δ_k sequences plotted versus k of $\Phi_{\infty}^{zz}(\omega)$ for four different parameter values. Between $J_z/J=0.6$ and $J_z/J = 1.0$, the sequence of known coefficients has a well defined growth rate somewhat in excess of $\lambda = 1$. For the XX model $(J_z=0)$, on the other hand, growth rate $\lambda=0$ is well known to be realized.^{5,23} The sequence for $J_z/J = 0.1$ has attributes of both regimes. It starts out with $\lambda = 0$ up to $k \simeq 7$ and then begins to grow with $\lambda \gtrsim 1$, thus causing a kink in Δ_k versus k. That is so throughout the range $0 < J_z/J < 0.6$. It is impossible to analyze such sequences on the basis of a unique value of λ , and, therefore, impossible to carry out the analysis described before without major modifications.³⁵

results presented in Sec. IV will further support the case

The bulk-spin spectral density $\Phi_{\infty}^{zz}(\omega)$ for four parameter values over the range $0.7 \le J_z/J \le 1.0$ as reconstructed from the 14 known Δ_k 's and a Gaussian terminator with its parameter from the Δ_k^* sequence is displayed in Fig. 6 (solid curves). Notice how the shape of the functions $\Phi_{\infty}^{zz}(\omega)$ (Fig. 6) and $\Phi_{\infty}^{xx}(\omega)$ (Fig. 3), which start out identically, undergo different changes as the anisotropy parameter decreases from $J_z/J=1$. While the function $\Phi_{\infty}^{xx}(\omega)$ gradually transforms into a pure Gaussian (dashed line in Fig. 3), the function $\Phi_{\infty}^{zz}(\omega)$ is supposed to approach the exact result¹⁷

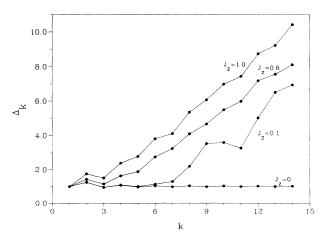


FIG. 5. Continued-fraction coefficients $\Delta_k^{zz}(\infty)$ vs k for the bulk-spin-autocorrelation function $\langle S_{\infty}^z(t)S_{\infty}^z \rangle$ at $T = \infty$ of the 1D $s = \frac{1}{2}$ XXZ model with J = 1 and $J_z = 0$ (XX case), $J_z = 0.1$, 0.6, and $J_z = 1.0$ (XXX case). The kink of the sequence for $J_z = 0.1$ illustrates the crossover between growth rates $\lambda = 0$ and $\lambda \ge 1$.

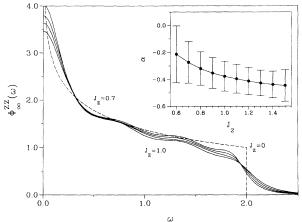


FIG. 6. Spectral density $\Phi_{\infty}^{zz}(\omega)$ at $T = \infty$ for the bulk-spin of the 1D $s = \frac{1}{2} XXZ$ model with J = 1 as reconstructed from the continued-fraction coefficients $\Delta_1^{zz}(\infty), \ldots, \Delta_{14}^{zz}(\infty)$ and a Gaussian terminator. The calculation was carried out by the use of the associated Δ_k^* sequence. The four solid curves represent the cases $J_z = 0.7, 0.8, 0.9, \text{ and } 1.0 (XXX \text{ model})$. The dashed curve is the exact result (5.1) for $J_z = 0$ (XX model). In the inset we have plotted the infrared-singularity exponent α vs J_z . The data points were obtained from $\Delta_3^{zz}(\infty), \ldots, \Delta_{14}^{zz}(\infty)$ by analyzing the Δ_k^* sequence.

$$\Phi_{\infty}^{zz}(\omega) = \frac{2}{\pi J} K(\sqrt{1 - \omega^2 / 4J^2}) \Theta(1 - \omega^2 / 4J^2) \quad (J_z = 0) .$$
(5.1)

The graph of that complete elliptic integral has been added as dashed line to Fig. 6. The diminishing height of the central peak with decreasing J_z/J marks the weakening of the divergence from $\sim \omega^{-1/2}$ (diffusive) to $\sim \ln(1/\omega)$ (free fermions). Spectral weight removed from the central peak and from the high-frequency tail is transferred to the shoulder, which gradually transforms into a discontinuity at $\omega/J = 2$.

The inset to Fig. 6 shows our results for the infrared singularity exponent α over the parameter range $0.6 \le J_z/J \le 1.5$. Within the statistical uncertainties indicated by error bars, the data points are consistent with a J_{z} -independent exponent. This confirms that the fluctuations of S_1^z are largely unaffected by the change in the symmetry at $J_{z}/J = 1$ in strong contrast to our observations made in Fig. 4 for the fluctuations of S_l^x . The weak monotonic J_z dependence of the mean exponent values at $J_{z}/J \ge 0.8$ and their deviation from the standard value $\alpha = -0.5$ are probably attributable to the previously mentioned systematic errors, which we have not fully under control. However the sloping tendency of the mean values toward the lowest values of J_z , and the extra large error bars on those data points are an artifact caused by the crossover between growth rates as discussed in the context of Fig. 5.

VI. BOUNDARY-SPIN SPECTRAL DENSITIES

The conclusions drawn in Secs. IV and V for the bulkspin spectral densities $\Phi_{\infty}^{xx}(\omega)$ and $\Phi_{\infty}^{zz}(\omega)$ are further substantiated when we look at the results of the same analysis carried out for the boundary-spin spectral densities $\Phi_0^{\mu\mu}(\omega)$, $\mu = x, z$. For that calculation we have 17 Δ_k 's at our disposal (compared to 14 in the bulk case), but the problem with the λ crossover now plagues both x and z fluctuations for parameters $0 \le J_z / J \le 0.6$.

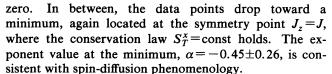
The spectral densities $\Phi_0^{xx}(\omega)$ for the cases $J_z/J=1.0, 0.6$ as reconstructed from the Δ_k^* sequence and a Gaussian terminator are shown in Fig. 7 (solid lines). The curve for the XXX case $(J_z=J)$ shows a pronounced peak at $\omega=0$. That conspicuous enhancement of spectral weight has all but disappeared for $J_z/J=0.6$, i.e., in the presence of anisotropy, where S_T^x is not conserved. Hence the central peak in the XXX result can again be interpreted as a spin-diffusive divergence.

As the anisotropy parameter is decreased below the value $J_z/J = 0.6$, the shape of the function $\Phi_0^{xx}(\omega)$ must approach that of the dashed line, which represents the exact result for $J_z/J = 0$, ^{22,23}

$$\Phi_0^{xx}(\omega) = (4/J)\sqrt{1 - \omega^2/J^2} \quad (J_z = 0) , \qquad (6.1)$$

which is the Fourier transform of $\langle S_0^x(t)S_0^x \rangle = [J_0(Jt) + J_2(Jt)]/4$. While the Δ_k^* analysis breaks down for small values of J_z/J , the way the function $\Phi_0^{xx}(\omega)$ develops between $J_z/J = 1.0$ and 0.6 can be extrapolated fairly smoothly toward the dashed line.

We have calculated the infrared-singularity exponent α of the boundary-spin spectral density $\Phi_0^{xx}(\omega)$ over the extended parameter range $0.6 \le J_z/J \le 1.2$ by means of the analysis explained previously. The inset to Fig. 7 shows seven equally spaced data points on that interval. The α values at the endpoints of the interval are very close to



Note the strongly contrasting J_z dependence of the singularity exponent pertaining to the spectral density $\Phi_0^{zz}(\omega)$ as shown in the inset to Fig. 8. Here the data points indicate the presence of an infrared divergence over the entire parameter range shown. However, a much stronger J_z dependence of the mean values of α is indicated than was the case of the corresponding bulk-spin results (Fig. 6). Whether that J_z dependence is entirely attributable to the systematic errors in our analysis and to the λ crossover remains to be seen.

In view of the fact that infrared divergences are likely to be real in the function $\Phi_0^{zz}(\omega)$ for all values of $J_z > 0$, we have treated them as such for its reconstruction from the known Δ_k 's. Instead of using a Gaussian terminator (cf. Sec. IV A), which is completely unbiased with respect to the spectral-weight distribution at low frequencies, we have used a two-parameter terminator with built-in infrared divergence. Its model relaxation function has been determined numerically via

$$\overline{c}(z) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega \frac{\overline{\Phi}(\omega)}{\omega - iz}$$
(6.2)

from the model spectral density (4.3) with $\lambda = 1$. The value of the parameter ω_0 is determined by the slope of Δ_k versus k as before and the parameter α by our estimate of the singularity exponent.

Two of the curves in the main plot of Fig. 8 represent

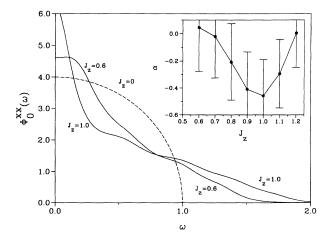


FIG. 7. Spectral density $\Phi_0^{xx}(\omega)$ at $T = \infty$ for the boundary spin of the semi-infinite 1D $s = \frac{1}{2} XXZ$ model with J = 1 as reconstructed from the continued-fraction coefficients $\Delta_1^{xx}(0), \ldots, \Delta_{17}^{xx}(0)$ and a Gaussian terminator. The calculation was carried out with the associated Δ_k^* sequence. The two solid curves represent the cases $J_z = 1.0$ (XXX model) and $J_z = 0.6$. The dashed curve is the exact result (6.1) for $J_z = 0$ (XX model). In the inset we have plotted the infrared-singularity exponent α vs J_z . The data points were obtained from $\Delta_5^{xx}(0), \ldots, \Delta_{17}^{xx}(0)$ by analyzing the Δ_k^* sequence.

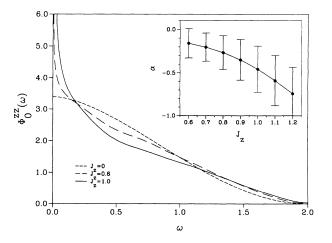


FIG. 8. Spectral density $\Phi_0^{zz}(\omega)$ at $T = \infty$ for the boundaryspin of the semi-infinite 1D $s = \frac{1}{2} XXZ$ model with J = 1 as reconstructed from the continued-fraction coefficients $\Delta_{12}^{zz}(0), \ldots, \Delta_{17}^{zz}(0)$ and a special terminator with built-in infrared divergence. The calculation was carried out with the associated Δ_k^* sequence for the two cases $J_z = 1.0$ (XXX model) and $J_z = 0.6$. Also shown is the exact result (6.3) for $J_z = 0$ (XX model). In the inset we have plotted the infrared-singularity exponent α vs J_z . The data points were obtained from $\Delta_{22}^{zz}(0), \ldots, \Delta_{17}^{zz}(0)$ by analyzing the Δ_k^* sequence.

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	13											134 217 728

TABLE I. Coefficients $m_{\mathbb{Z}_{k}}^{\mathbb{Z}_{k}}(\infty, 2n)$ of the expansion (A1).

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					IA	ABLE II. Coeffic	tents $m_{2k} (\infty, 2n)$	ABLE II. Coefficients $m_{2k}^{\infty}(\infty, 2n)$ of the expansion (A1)	A1).		
4							(a)				
v u	0		2	Э	4	5	9	7	8	6	10
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e				32	1792	63 744	1 953 776	56 926 012	1 645 089 888	49 127 454 896	1 650 071 143 616
4					128	11 520	663 872	31 787 392	1 384 501 248	57 265 586 368	2 314 444 556 752
5						512	67 584	6 456 320	490 989 056	31 918 392 704	1 884 787 750 016
9							2 048	372 736	65 516 544	8 028 291 072	762 099 244 032
٢								8 192	1 966 080	753 139 712	143 168 688 128
8									32 768	10 027 008	9 966 141 440
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3		71	71 440 014 187 376	7 376		4 224 665 438 128 064	128 064	306 44	306 448 398 158 942 240	24 02	24 028 691 547 335 252 400
4		94	94 831 675 835 968	5 968		4 249 623 524 974 624	974 624	23578	235 784 156 426 515 200	17.37	17 376 963 387 911 026 200
2		105	105 259 016 639 040	9 040		5 715 363 282 918 656	918 656	31098	310 980 152 826 272 160	16.21	17 917 127 977 298 169 600
9		62	62 721 972 915 712	5712		4 772 749 197 832 832	832 832	347 31	347 319 490 135 290 880	24 68	24 683 103 277 934 568 960
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10			242 221 056	1 056		2 247 649 132 544	132 544	100	1 005 690 153 861 120	26	262 983 884 215 418 880
11			2 09	097 152		1 157	1 157 627 904	(*)	35 458 729 902 080	1	19 188 697 927 778 304
12						œ	8 388 608		5 452 595 200		564 456 232 845 312
13									33 554 432		25 367 150 592
14											134 217 728

TABLE II. Coefficients $m_{2k}^{xx}(\infty, 2n)$ of the expansion (A1).

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BÖHM, VISWANATH, STOLZE, AND MÜLLER

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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	9		79 551 .	764 550 48	0	2 913 957 29	7 036 015	1048	95 736 359 160 905		09 454 596 717 102 08	-	129 278 403 677 771 856 300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	٢		38 257 .	727 114 94	0	1 810 145 26.	3 080 690	827	30 076 297 083 385		70 990 174 588 316 70	-	59 085 198 123 172 037 048
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	×		10 055 4	195 062 50	0	635 171 77.	3 479 930	374	49 331 649 060 445		93 100 135 486 779 76		112 327 113 474 260 368 824
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6		1 399 {	325 120 58	0	126488150	6 851 605	100	25 102 368 543 713		22 421 733 226 903 82	•	48 591 706 611 682 667 464
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10		916	75 566 66	5	13 549 52	8 822 377	15	64 366 561 926 945		52 179 442 064 682 48		13 181 808 438 206 934 780
33 554 587 10 804 550 050 5 097 573 875 065 1 322 1 134 217 909 50 331 678 465 40 1 536 871 121 1 1	11		22	90 106 89	7	670 34	7 869 790	1	32 967 383 212 721		19 097 204 936 013 83		2 235 049 510 341 476 016
1 134217909 50331678465 40 1 536871121 1	12			33 554 58'	7	1080	4 550 050		5 097 573 875 065		1 322 567 599 253 08	2	230 208 596 780 129 760
1 536 871 121 1	13			·	1	13-	4 217 909		50 331 678 465		40 527 104 759 75		13 282 222 997 574 528
	14						1		536 871 121		231 928 273 68	0	335 075 020 631 015
16 17	15								1		2 147 483 88	1	1 058 709 489 345
1	16											1	8 589 934 863
	17												-

(T A 1)

the function $\Phi_0^{zz}(\omega)$ for $J_z/J=1.0$ and $J_z/J=0.6$ as reconstructed form the 17 known continued-fraction coefficients and this special terminator. As the parameter drops from the higher to the lower value, the central peak in the spectral density weakens considerably, and the weak shoulder at $\omega=J$ present for $J_z/J=1.0$ all but disappears. Upon further decrease of J_z/J to zero (XX model), the curve is supposed to approach the dashed line, which is the known exact result²³

$$\Phi_0^{zz}(\omega) = \frac{128}{3\pi J} (1 + \omega/2J) \left[(1 + \omega^2/4J^2) E\left(\frac{2J - \omega}{2J + \omega}\right) - \frac{\omega}{J} K\left(\frac{2J - \omega}{2J + \omega}\right) \right].$$
(6.3)

This limiting case is perfectly in line with how the reconstructed spectral density develops between $J_z/J = 1.0$ and $J_z/J = 0.6$.

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APPENDIX A

The frequency moments (2.2) of the spectral density (1.3) as expressed in terms of the expectation values (2.3) yield upon evaluation, for the *XXZ* model (1.1), expressions of the form

$$M_{2k}^{\mu\mu}(l) = 2^{-2k} \sum_{n=0}^{k} m_{2k}^{\mu\mu}(l,2n) J_{z}^{2n} J^{(2k-2n)}$$
(A1)

with integer coefficients $m_{2k}^{\mu\mu}(l,2n)$. We have computed these coefficients up to k = 14 for the bulk spin $(l = \infty)$ and up to k = 17 for the boundary spin (l = 0). The former are listed in Table I for $\mu = z$ and Table II for $\mu = x$, the latter in Table III for $\mu = z$ and Table IV for $\mu = x$.

APPENDIX B

The first K expansion coefficients M_{2k} , k = 1, ..., K of an autocorrelation function (1.2) (or frequency moments of its Fourier transform) determine the first K continuedfraction coefficients Δ_k , k = 1, ..., K of its Laplace transform (2.4) and vice versa. The Δ_k , for example, are expressible in terms of Hankel determinants with elements consisting of moments M_{2k} .^{5,36,37} There exist several different algorithms for the numerical conversion of one set of numbers into the other. Some of them are more susceptible to numerical instabilities than others.³⁷ The following algorithm,³⁸ which is a product of the recursion method, has proven to be fairly robust against numerical instabilities in our applications:

Forward direction: For a given set of moments M_{2k} , k = 0, 1, ..., K with $M_0 = 1$, the first K coefficients Δ_m , are determined by

$$\boldsymbol{M}_{2k}^{(m)} = \frac{\boldsymbol{M}_{2k}^{(m-1)}}{\Delta_{m-1}} - \frac{\boldsymbol{M}_{2k-2}^{(m-2)}}{\Delta_{m-2}}, \quad \Delta_m = \boldsymbol{M}_{2m}^{(m)}$$
(B1)

for k = m, m + 1, ..., K and m = 1, 2, ..., K and with set values $M_{2k}^{(0)} = M_{2k}, \Delta_{-1} = \Delta_0 = 1, M_{2k}^{(-1)} = 0.$

Reverse direction: For a given set of $\Delta_m = M_{2m}^{(m)}$, m = 1, ..., K, and $\Delta_{-1} = \Delta_0 = 1$, the moments $M_{2n}^{(0)} = M_{2n}$, result from the relations,

$$M_{2k}^{(m-1)} = \Delta_{m-1} M_{2k}^{(m)} + \frac{\Delta_{m-1}}{\Delta_{m-2}} M_{2k-2}^{(m-2)}$$
(B2)

for m = k, k - 1, ..., 1 and k = 1, 2, ..., K and with set values $M_{2k}^{(-1)} = 0$.

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- ³³What looks like a gradual increase of λ may, in fact be a crossover between two fixed values of growth rate, one for free fermions (λ =0) and another one for interacting fermions (λ ~1.2). What counts for our analysis is the effective growth rate pertaining to the known finite Δ_k sequence.
- ³⁴It is no problem to design adjustments that remove some of the most obvious systematic errors in the results presented in Secs. IV-VI and to justify these corrections by very reasonable arguments. However, there is some ambiguity in how to implement these adjustments. This makes it hard to fully detach the choice of implementation from hindsight knowledge. We have decided, therefore, to present our results here without any such adjustments for systematic errors.
- ³⁵If the kink occurs at sufficiently large values of k, one might be tempted to analyze that Δ_k sequence on the basis of $\lambda=0$. The problem is that the interesting physics, caused by the effects of the fermion interaction for the case at hand, is contained in the Δ_k past the kink. Therefore, not much may be gained by such an exercise.
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