

## Spin diffusion and the spin-1/2 XXZ chain at $T = \infty$ from exact diagonalization

Klaus Fabricius\*

*Physics Department, University of Wuppertal, 42097 Wuppertal, Germany*

Barry M. McCoy†

*Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794-3840*

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We study the long time behavior of the  $zz$  and  $xx$  time-dependent autocorrelation function of the spin-1/2 XXZ chain at  $T = \infty$  by exact diagonalizations on a chain of 16 sites. We find that the numerical results for the  $zz$  correlation are very well fit by the formula  $t^{-d}[A + B e^{-\gamma(t-t_0)} \cos \Omega(t-t_0)]$ . From this we estimate  $d$  as a function of the anisotropy of the chain and study the crossover from ballistic to diffusive behavior. [S0163-1829(98)06014-7]

### I. INTRODUCTION

The phenomenological theory of spin diffusion was proposed by Bloembergen<sup>1</sup> and de Gennes<sup>2,3</sup> to give a description of inelastic neutron scattering in magnetic systems at elevated temperatures. It is based on the physical argument that at high enough temperatures the modes of the system become independent and may be represented as Gaussian fluctuations. The argument is independent of dimension and one of the elementary consequences of this theory is that at infinite temperature the autocorrelation of a spin which obeys a conservation law has the long-time behavior in dimension  $d$

$$S(t) \sim A t^{-d/2}. \quad (1.1)$$

This spin-diffusion phenomenology is extensively used to study neutron scattering in real magnetic systems.<sup>4</sup>

It is of considerable interest to demonstrate that this phenomenology follows in some degree of universality for a large class of conservative systems specified by a Hamiltonian and over the years there have been a variety of arguments made for its validity.<sup>5-8</sup> In parallel to these investigations there has been a long series of attempts to find a system sufficiently simple to actually compute an autocorrelation function and to then see whether or not the spin-diffusion behavior actually holds. Most of the studies have been in one dimension where the long-time dependence of Eq. (1.1) is

$$S(t) \sim A t^{-1/2}. \quad (1.2)$$

The most studied quantum-mechanical model is the spin-1/2 XXZ chain of  $N$  sites with periodic boundary conditions specified by the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z), \quad (1.3)$$

where  $\sigma_i^j$  is the  $j=x,y,z$  Pauli spin matrix at site  $i$ . The autocorrelation functions at infinite temperature are defined as

$$S^j(t; \Delta) = \langle \sigma_0^j(t) \sigma_0^j(0) \rangle = \lim_{N \rightarrow \infty} 2^{-N} \text{Tr} e^{-itH} \sigma_0^j e^{itH} \sigma_0^j. \quad (1.4)$$

These correlations have been studied for the isotropic case  $\Delta = 1$  by numerical and approximation methods for over 30 years.<sup>9-19</sup>

What is very surprising is that after so much effort the answer to the question of whether or not there is spin diffusion in the XXZ model has not been resolved (see Chap. 10 of Ref. 18 for a detailed discussion of the situation as of 1994). This is all the more surprising since the spin-1/2 XXZ model is the oldest known solvable spin chain. However, after decades of effort the only exact results known for the autocorrelation at  $T = \infty$  Eq. (1.4) are as follows:

(1) The general result proven in Ref. 20 (with a mild assumption) that the Fourier transform  $\tilde{S}^z(\omega, \Delta)$  of  $S^z(t, \Delta)$  must diverge when  $\omega \rightarrow 0$  at least as rapidly as  $\ln \omega^{-1}$  and that if the asymptotic behavior Eq. (1.2) holds then as  $\omega \rightarrow 0$

$$\tilde{S}^z(\omega) \sim A' \omega^{-1/2}, \quad (1.5)$$

and

(2) the results specific to  $\Delta = 0$  that<sup>21</sup>

$$S^z(t; 0) = [J_0(2t)]^2 = \left[ \frac{1}{\pi} \int_0^\pi \cos 2t \sin \theta d\theta \right]^2 \quad (1.6)$$

where  $J_0(2t)$  is the Bessel function of order zero and<sup>22-24</sup>

$$S^x(t, 0) = e^{-t^2}. \quad (1.7)$$

The total spin component  $\sum_{i=0}^N \sigma^x$  will only commute with  $H$  if  $\Delta = 1$  and hence in general depends on time. Thus  $S^x(t, \Delta)$  is not expected to have spin-diffusion behavior for  $\Delta \neq 1$ . However  $\sum_{i=1}^N \sigma_i^z$  does commute with  $H$  and hence does satisfy the conservation law needed for spin diffusion. Nevertheless for large  $t$  we see from Eqs. (1.6) that  $S^z(t; 0)$  behaves as

TABLE I. The best fit parameters for the system with  $N=16$  spins. The entries  $t_1$  and  $t_2$  indicate the time interval for which the fit (3.1) is good.

$\Delta$	$d$	$A$	$B$	$\gamma$	$\Omega$	$t_0$	$t_1$	$t_2$	$\chi^2$
0.0	1.000	0.159	0.159	0.000	4.010	1.976	2.5	5.0	1.199e-07
0.1	0.961	0.156	0.153	0.023	4.009	1.977	2.5	5.0	1.651e-07
0.2	0.875	0.152	0.141	0.083	4.007	1.976	2.5	5.0	1.520e-07
0.3	0.810	0.156	0.131	0.159	4.007	1.976	2.5	5.0	1.071e-08
0.4	0.835	0.180	0.127	0.217	4.039	1.985	3.0	5.8	1.016e-06
0.5	0.912	0.219	0.120	0.246	4.080	1.987	3.5	6.0	7.327e-08
0.6	0.941	0.246	0.108	0.290	4.138	1.987	3.5	6.0	1.659e-07
0.7	0.902	0.251	0.092	0.361	4.213	1.989	3.1	6.0	4.273e-06
0.8	0.840	0.249	0.079	0.453	4.274	1.973	3.1	6.0	5.789e-07
0.9	0.771	0.248	0.066	0.558	4.353	1.958	3.0	5.7	2.165e-07
1.0	0.705	0.247	0.053	0.668	4.439	1.933	3.2	5.1	4.202e-10
1.1	0.646	0.249	0.041	0.775	4.568	1.906	3.0	4.5	9.062e-11
1.2	0.602	0.254	0.027	0.811	4.779	1.866	3.0	4.5	8.756e-11
1.3	0.572	0.263	0.015	0.669	5.010	1.769	3.0	4.5	8.568e-11

$$S^z(t;0) \sim \frac{1}{\pi t} \cos^2\left(2t - \frac{\pi}{4}\right) = \frac{1}{2\pi t} \left[1 + \cos\left(4t - \frac{\pi}{2}\right)\right], \quad (1.8)$$

which is certainly not of the form (1.2).

In the absence of exact computations recourse has been made to a variety of speculations. For example,<sup>25,26</sup> it may be argued that the reason the XXZ model is solvable in the first place is because it possesses an infinite number of conservation laws and that this violates the assumption of independence of modes used in Refs. 2,3. This would argue that there is no reason that there should ever be spin diffusion in the model.

One can also attempt to gain inspiration from low-temperature and field theory limit computations. As far back as Ref. 11 and most recently in Ref. 27, it is argued that at low temperature there is no spin diffusion for  $-1 \leq \Delta \leq 1$ , where there is no long-range order at  $T=0$ . However, from a low-temperature computation of Sachdev and Damle<sup>28,29</sup> it can be argued that for  $1 < \Delta$ , where there is long-range order

at  $T=0$ , spin diffusion will hold. Thus, as a possibility, it can be suggested that for the spin-1/2 XXZ model there could be a nonanalytic behavior at  $\Delta=1$  such that at  $T=\infty$  there would be spin diffusion for  $\Delta > 1$  and no spin diffusion for  $0 \leq \Delta \leq 1$ .

In this paper we assess the merits of these suggestions by an extension of the work of Ref. 19. In particular for a spin chain of size  $N=16$  we compute exactly by diagonalizing the finite-size matrices the spin-correlation functions (1.4). These results are given in Sec. II. We then analyze these results in Sec. III in terms of the ansatz on the long-time behavior of Ref. 13 and conclude with a discussion in Sec. IV.

The conclusion of this analysis as given in Tables I and II is that we do indeed see evidence for  $0 \leq \Delta \leq 1$  that spin diffusion does not hold. Indeed it is consistent with our data that as  $t \rightarrow \infty$

$$S^z(t,\Delta) \sim A/t \quad \text{for } 0 \leq \Delta < 1, \quad (1.9)$$

TABLE II. The best fit parameters for the system with  $N=14$  spins. The entries  $t_1$  and  $t_2$  indicate the time interval for which the fit (3.1) is good.

$\Delta$	$d$	$A$	$B$	$\gamma$	$\Omega$	$t_0$	$t_1$	$t_2$	$\chi^2$
0.0	0.985	0.156	0.157	0.006	4.015	1.978	2.0	4.0	4.283e-08
0.1	0.954	0.155	0.153	0.028	4.013	1.978	2.0	4.0	2.255e-08
0.2	0.882	0.154	0.142	0.085	4.008	1.977	2.0	4.0	1.474e-09
0.3	0.809	0.156	0.131	0.158	4.006	1.975	2.0	4.0	1.552e-09
0.4	0.784	0.168	0.123	0.231	4.013	1.973	2.5	4.8	1.653e-07
0.5	0.833	0.196	0.123	0.301	4.055	1.979	2.8	5.0	5.627e-07
0.6	0.885	0.227	0.114	0.348	4.134	1.990	3.0	5.2	4.273e-07
0.7	0.840	0.230	0.103	0.446	4.145	1.960	2.5	5.1	9.297e-06
0.8	0.801	0.236	0.086	0.515	4.210	1.948	2.5	5.0	2.759e-06
0.9	0.746	0.239	0.071	0.599	4.285	1.932	2.5	4.8	5.122e-07
1.0	0.694	0.244	0.056	0.692	4.403	1.922	2.8	4.5	4.914e-09
1.1	0.640	0.247	0.041	0.773	4.536	1.895	2.6	4.0	5.642e-11
1.2	0.608	0.256	0.027	0.821	4.804	1.875	2.6	4.0	2.236e-10
1.3	0.577	0.265	0.015	0.654	5.025	1.774	3.0	4.0	4.089e-12

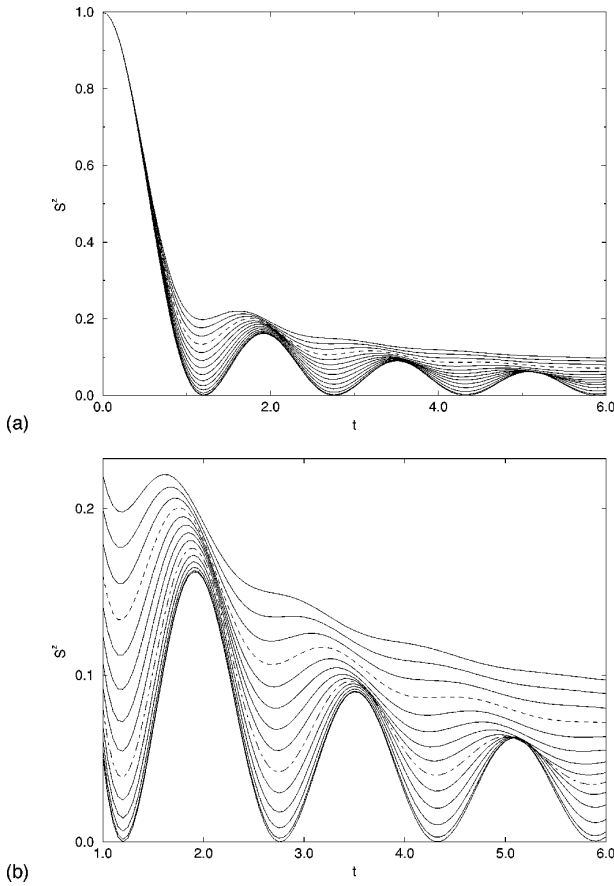


FIG. 1. (a) The correlation function  $S^z(t, \Delta)$  as computed from the  $N=16$  spin chain for  $0 \leq \Delta \leq 1.3$  in steps of 0.1. On this scale the curves are monotonic functions of  $\Delta$  with  $\Delta=0$  lying lowest. The curve for  $\Delta=1$  is dashed. (b) The correlation function  $S^z(t, \Delta)$  of (a) on the time range  $1 \leq t \leq 6$ . The curve for  $\Delta=1$  is dashed and for  $\Delta=0.5$  is dot dashed. On this scale we see that near  $t=5.0$  that for  $0 \leq \Delta \leq 0.5$  there is crossing of the curves.

which is the same as the ballistic behavior of the  $\Delta=0$  (free fermion case). Moreover at  $\Delta=1$  we find strong evidence supporting the behavior

$$S^z(t, 1) \sim A/t^{0.705}, \quad (1.10)$$

which is neither ballistic nor diffusive. This result is in agreement with the estimate of Ref. 18 that  $\bar{S}^z(\omega)$  diverges as  $\omega^{-0.37 \pm 0.12}$  as  $\omega \rightarrow 0$ . For  $\Delta > 1$  we cannot be so positive as to whether or not spin diffusion exists and we defer further discussion to the end of Sec. III.

### II. FINITE-SIZE RESULTS FOR $N=16$

We have evaluated  $S^z(t, \Delta)$  for chains up to size  $N=16$  using the methods of exact diagonalization presented in Ref. 19. We plot our results for  $0 \leq \Delta \leq 1.3$  in steps of 0.1 in Fig. 1. The results presented here extend the previous work principally in that data is used which range over a larger time interval and many more values of  $\Delta$  have been studied.

Data on finite-size systems will only well approximate infinite-size systems for some finite time interval. In Ref. 19 the criteria used was that the data for  $N=14$  and  $N=16$  should closely agree. This amounts to using the  $N=16$  data

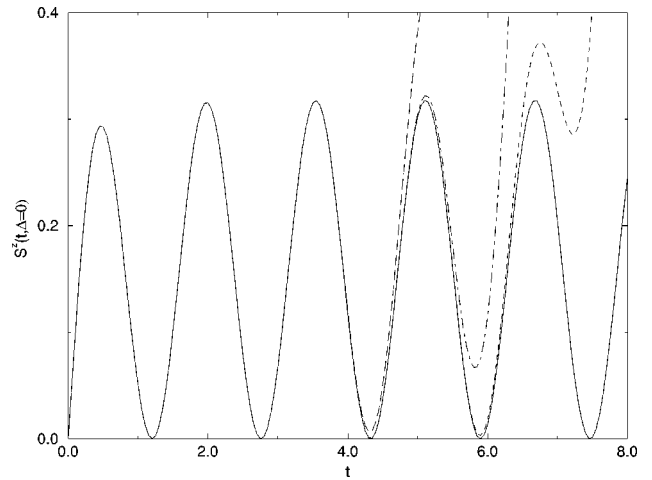


FIG. 2. Comparison of the exact result  $1.6 t S^z(t, 0)$  (solid line) with the finite-size computations for  $N=12$  (long dashes),  $N=14$  (dot dashes), and  $N=16$  (short dashes).

to tell us how much of the  $N=14$  data can be used. However the  $N=16$  data will agree with the  $N=\infty$  curve for a longer time interval. We estimate this larger interval in two ways. First by comparing the exact result (1.6) for  $\Delta=0$  with the finite-size result for  $N=16$ . The second is by making an

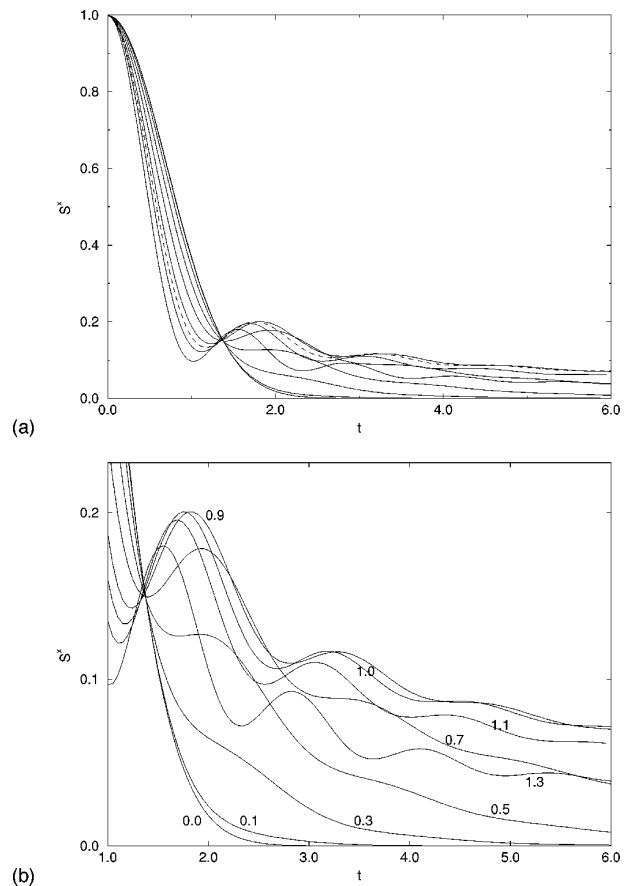


FIG. 3. (a) The correlation function  $S^x(t, \Delta)$  as computed from the  $N=16$  spin chain for the values  $\Delta=0.0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 1.1,$  and  $1.3$ . The curve  $\Delta=1$  is dashed and for  $0 \leq t \leq 1.2$  the curves are monotonic in  $\Delta$  with  $\Delta=0$  lying highest. (b) The correlation function  $S^x(t, \Delta)$  of (a) on the time interval  $1 \leq t \leq 6$ . The values of  $\Delta$  are indicated on the curves.

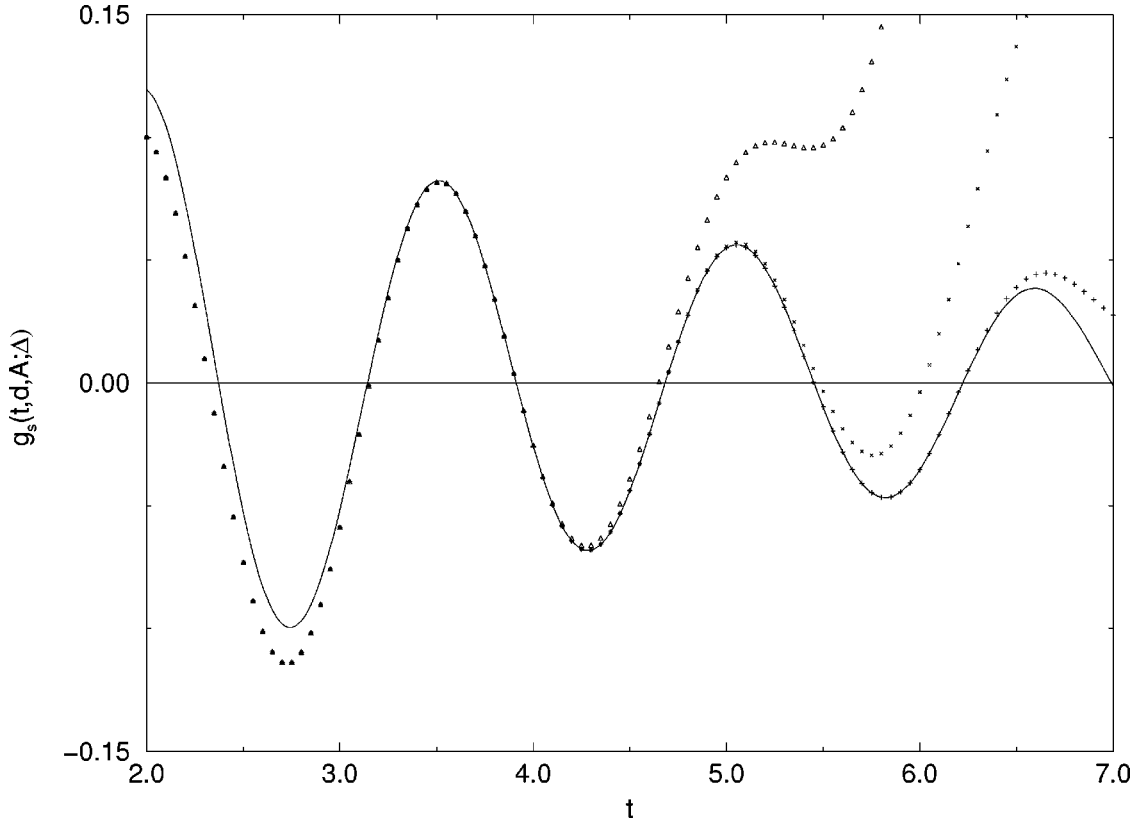


FIG. 4. Least-squares fit (solid line) of the  $N=16$  data (vertical crosses) for  $S^z(t, \Delta)$  in the form (3.3) to the form (3.2) for  $\Delta=0.5$ . The values of the parameters are  $d=0.912$ ,  $A=0.219$ ,  $B=0.120$ ,  $\gamma=0.246$ ,  $\Omega=4.080$ ,  $t_0=1.987$ , and the interval of best fit is  $3.5 < t < 6.0$ . The data for  $N=14$  (diagonal crosses) and  $N=12$  (triangles) are also shown.

extrapolation using the data for  $N=12, 14$ , and  $16$ . We make these comparisons in Fig. 2 for  $\Delta=0$ . This allows us to effectively extend the range of  $t$  from  $t_{\max}=5.0$  which was what was used in Ref. 19 to  $t_{\max}=6$  or greater in some cases. The maximum time is estimated for each  $\Delta$  separately, since with the normalization of Eq. (1.3) the maximum time will decrease as  $\Delta$  increases. It is possible to introduce a normalization which makes  $t_{\max}$  relatively independent of  $\Delta$  but since this is somewhat *ad hoc* and arbitrary we will not do this here.

We have also made a similar study for the correlation  $S^x(t; \Delta)$ . These results are presented graphically in Fig. 3.

There are two qualitative features of these graphs which should be noted. First of all in the graph for  $S^x(t, \Delta)$  the long-time behavior of  $\Delta=1$  lies higher than all other values of  $\Delta$ . This is expected from fact that if  $\Delta=1$  then  $S^x(t) = S^z(t)$  and thus the long-time behavior must be algebraic which is to be contrasted with the exponential decay expected for all other values of  $\Delta$  where there is no conservation of  $\sum_j \sigma_j^x$ . However near  $t=6.0$  the curves for  $\Delta=0.9$  and  $\Delta=1.0$  are so very close that this change in asymptotic behavior cannot yet be seen in the data.

The other point to note is that in Fig. 1(b) we see clearly that near  $t=5.0$  there is crossing of curves for  $0 \leq \Delta \leq 0.5$ . This effect is real and is not an artifact of the size  $N=16$ . We interpret this as evidence that if  $0 \leq \Delta \leq 0.5$  then  $t$  must be greater than  $5.0$  before the true long-time asymptotic regime is seen. In other words we take this as evidence that there is a crossover in the system.

### III. ASYMPTOTIC FITTING

In order to analyze the existence of spin diffusion we must extract the long-time behavior of the correlation function  $S^z(t, \Delta)$ . It is obvious from Fig. 1 that for times up to  $t=6$  that there are oscillations in the data and that a simple power law will not be adequate to describe the results. Here we confront this problem by fitting the curves with an extension of the simple ansatz proposed in Ref. 13 which incorporates a decaying oscillation as well as a decay with an arbitrary power law

$$f(t; d, A, B, \gamma, \Omega, t_0) = t^{-d} [A + B e^{-\gamma(t-t_0)} \cos \Omega(t-t_0)]. \quad (3.1)$$

In Figs. 4, 5, and 6 we illustrate this fitting procedure by showing a least-squares fit of

$$g_f(t; B, \gamma, \Omega, t_0) = B e^{-\gamma(t-t_0)} \cos \Omega(t-t_0) \quad (3.2)$$

to the function obtained from the  $N=16$  data of Fig. 1

$$g_s(t, d, A; \Delta) = t^d S^z(t; \Delta) - A \quad (3.3)$$

for the values  $\Delta=0.5, 1.0$ , and  $1.3$ .

More systematically we present in Table I the parameters of the form (3.1) which best fit all the data with  $N=16$  presented in Fig. 1 and the time intervals over which the fit is valid. In Table II we give the corresponding fitting parameters and time intervals for the data with  $N=14$ . We note from Eq. (1.8) that at  $\Delta=0$  the exact values of the parameters are

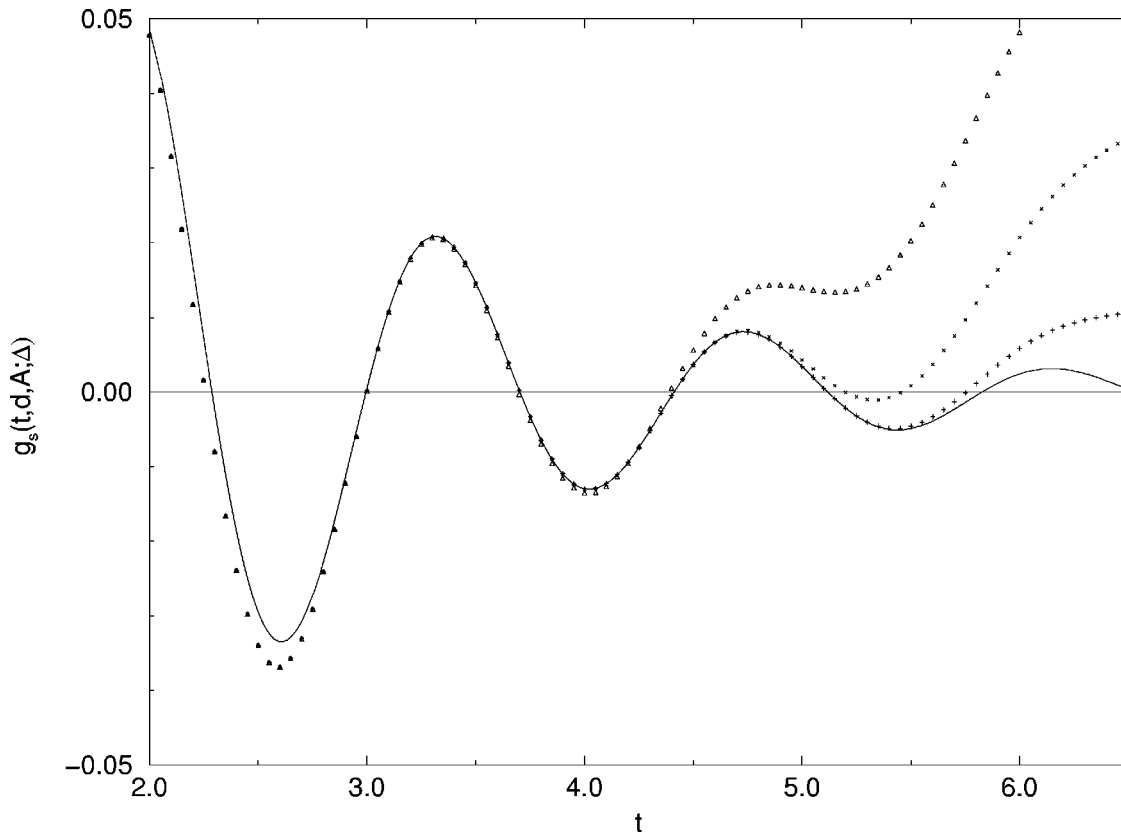


FIG. 5. Least-squares fit (solid line) of the  $N=16$  data (vertical crosses) for  $S^z(t, \Delta)$  in the form (3.3) to the form (3.2) for  $\Delta=1.0$ . The values of the parameters are  $d=0.705$ ,  $A=0.247$ ,  $B=0.053$ ,  $\gamma=0.668$ ,  $\Omega=4.439$ ,  $t_0=1.933$ , and the interval of best fit is  $3.2 < t < 5.1$ . The data for  $N=14$  (diagonal crosses) and  $N=12$  (triangles) are also shown.

$$d=1 \quad A=B=1/2\pi=0.159155\dots, \quad \gamma=0, \quad \Omega=4.0,$$

$$t_0=5\pi/8=1.9635\dots \quad (3.4)$$

It is very instructive to compare the values of the fitting parameters as obtained in the two tables. For  $\Delta=0$  and 1 the values of  $d$  changes little in going from  $N=14$  to  $N=16$ . But this is not the case for all values of  $\Delta$  and we compare the cases  $N=14$  and  $N=16$  in Fig. 7. First of all we see that for  $0.4 \leq \Delta \leq 0.9$  there is a great deal of variation in  $d$  as we go from  $N=14$  to  $N=16$ . We interpret this as an indication that there is a crossover in the behavior from small to large times. We expect that as  $N$  increases this trend will continue for all  $0 < \Delta < 1.0$  and eventually the data for  $0 < \Delta < 0.4$  will be affected also. We cannot definitively say from these plots what the true value of  $d$  will be for  $N \rightarrow \infty$  but because the fitted value of  $d$  is increasing in our tables for  $0 < \Delta < 1$  we conclude that the spin-diffusion value of  $1/2$  is never attained. At  $\Delta=1$  the value  $d=0.705$  is seen to be quite stable and we note that to within our accuracy it is equal to  $2^{-1/2}$ . From our analysis  $d$  could either be a continuous function of  $\Delta$  at  $\Delta=1$  or we could have  $d=1$  for  $0 \leq \Delta < 1$ .

For  $1 < \Delta$  we cannot be so positive in our conclusion. For  $\Delta=1.2, 1.3$  the fitted values of  $d$  do indeed decrease as  $N$  goes from 14 to 16 and it is not out of the question that as  $N \rightarrow \infty$  the limiting value could be  $1/2$  for all values of  $1 < \Delta$ . However this is not mandated by our results.

#### IV. DISCUSSION

The conclusion of the previous section is that in the spin- $1/2$  XXZ model specified by Eq. (1.3) there is no spin diffusion for  $0 \leq \Delta \leq 1$ . This needs to be discussed both as to its correctness and its implications.

We first acknowledge that it is possible to make contradictory suggestions as to what is to be expected and that different authors seem to implicitly start from different conceptions of what is going on. For example, the authors in the mid 1960s speak of their work as the hydrodynamic approximation and thus is sometimes said to be inapplicable to one and two dimensions where the Fourier transform of the autocorrelation function diverges. This would argue that one dimension always needs a separate treatment. However, most of the more recent authors seem to write as if the diffusion form (1.2) is to be expected in one dimension if only in the fact that deviations from it are called ‘‘anomalous.’’

Indeed, the question of whether or not this anomalous diffusion occurs in the classical one-dimensional Heisenberg model has been a subject of some controversy in the past 10 years.<sup>30–35</sup> It is agreed by all that for times up to about 50 an exponent of  $d \sim 0.61$  can be obtained from computer simulations. What is controversial is the ultimate long-time behavior. The arguments are summarized in Ref. 18. What is important for us here is to note that for the spin- $1/2$  quantum-mechanical case it is not possible with current computing power to go to anything approaching the large time of these classical computations. Thus all speculations and conjectures

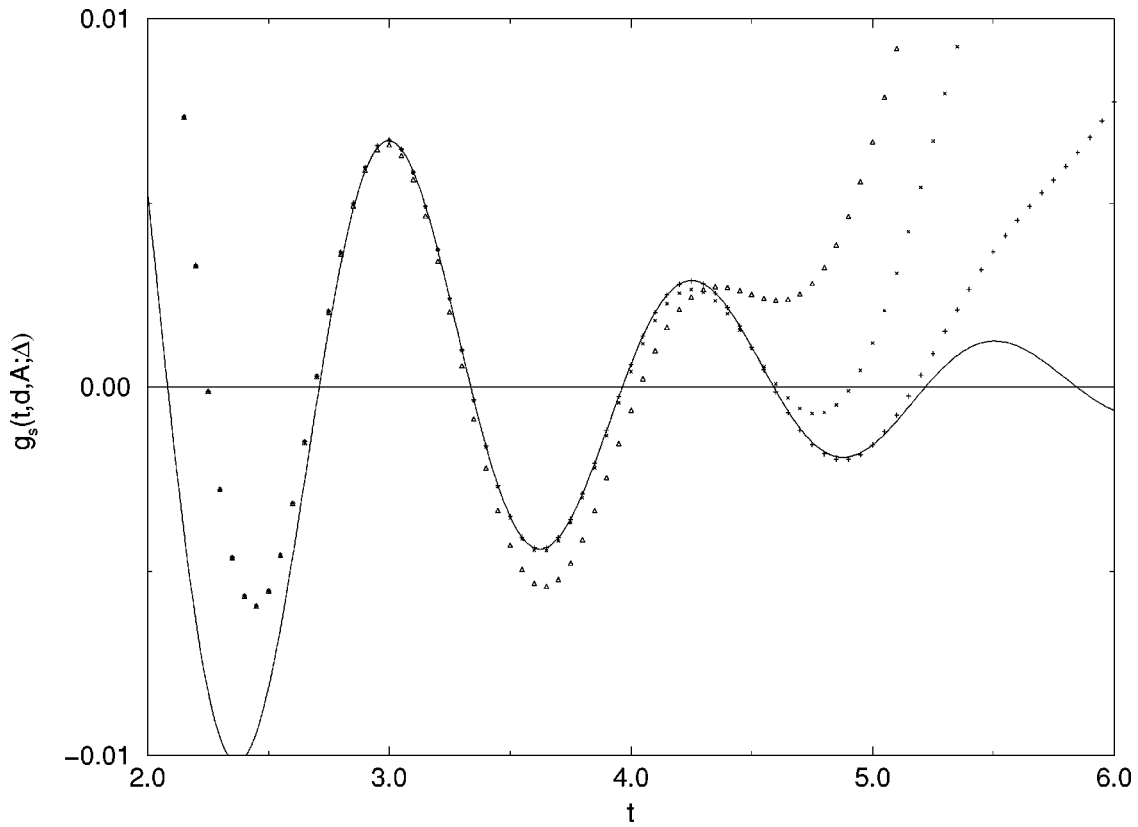


FIG. 6. Least-squares fit (solid line) of the  $N=16$  data (vertical crosses) for  $S^z(t, \Delta)$  in the form (3.3) to the form (3.2) for  $\Delta=1.3$ . The values of the parameters are  $d=0.572$ ,  $A=0.263$ ,  $B=0.015$ ,  $\gamma=0.669$ ,  $\Omega=5.010$ ,  $t_0=1.769$ , and the interval of best fit is  $3.0 < t < 4.5$ . The data for  $N=14$  (diagonal crosses) and  $N=12$  (triangles) are also shown.

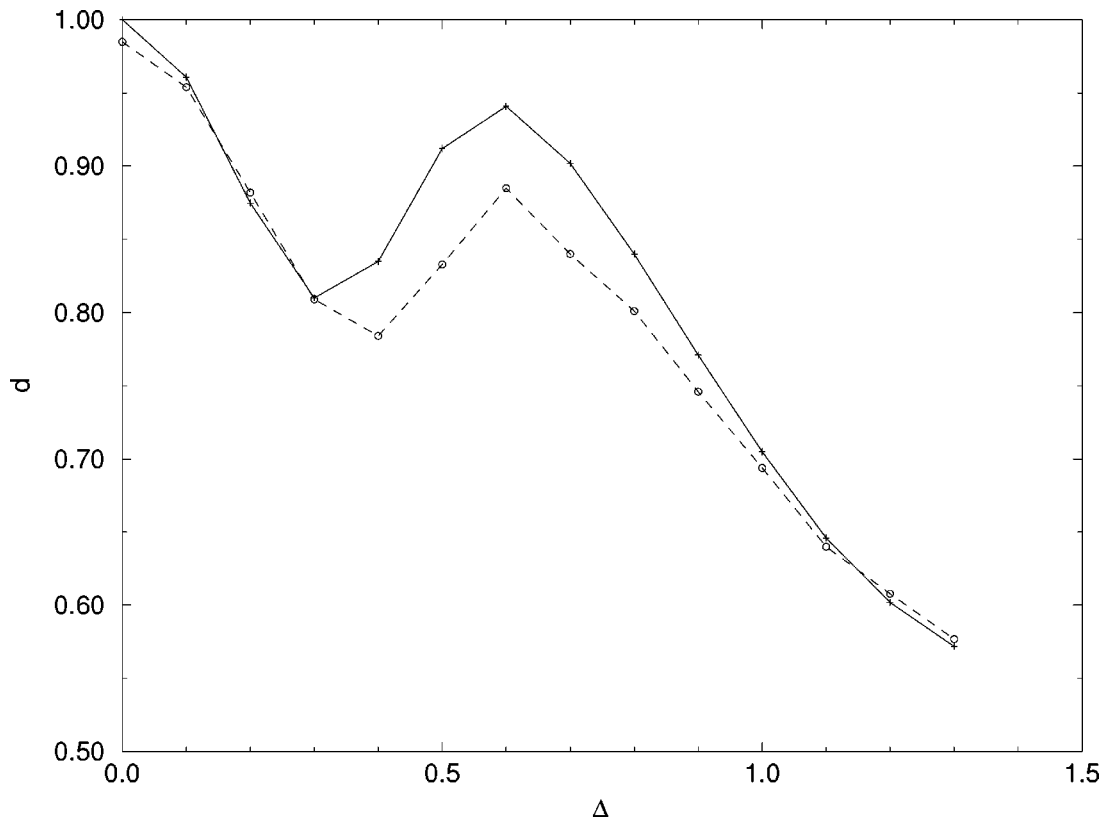


FIG. 7. Comparison of the best fit values of  $d$  for  $N=14$  and  $N=16$ .

about the long-time behavior of the spin-1/2 model are subject to the proviso that we assume that times up to  $t=6$  are able to teach us about the true  $t \rightarrow \infty$  behavior. It is our belief that the integrability of the spin-1/2  $XXZ$  chain will rule out the possibility of a new time scale appearing for large times but there is no way of verifying this short of an exact computation.

If it is accepted that the estimate of the asymptotic behavior we have presented here is indeed correct for the model (1.3) it must then be asked whether or not this is generic in any sense. It is here that the question of the relation of an integrable to a generic system needs to be addressed.

In the first place there is ample computer evidence<sup>36</sup> that if a sufficiently strong next-nearest-neighbor interaction is added to Eq. (1.3) then the level spacing statistics will change from Poisson for Eq. (1.3) to those of the Gaussian orthogonal ensemble of random matrices. It thus might be supposed that this will change the long-time behavior of the correlation functions. We have indeed looked at this in the  $N=16$  system but find that the asymptotic behavior up to time  $t=6$  does not change. But, of course, this proves little or nothing since if a scale is opened up at larger times the  $N=16$  system can hardly be expected to see it. It is certainly possible that all the complications seen in the classical system can occur for the nonintegrable quantum spin chain if we could go to large enough times. This is the place where ideas of quantum chaos should be able to intersect many-body condensed matter physics.

We also comment further on our suggestion of nonanalytic behavior at  $\Delta=1$ . It is of course perfectly reasonable that at  $T=0$  there will be a marked difference in the physics of  $0 \leq \Delta \leq 1$  and  $1 < \Delta$ . In the first case there is no long-range order and no gap in the spectrum, while in the second case there is both long-range order and a gap in the spectrum.<sup>37,38</sup> It is exactly these qualitative differences which feature in the low-temperature computations of Refs. 27, 28, and 29. But at high temperature it seems unreasonable that

such low-temperature properties as whether or not there is a gap in the excitations above the ground state should make any difference. It would seem that to maintain that there is nonanalytic behavior at  $\Delta=1$  we must violate our physical intuition.

The resolution to this would seem to lie in the integrability of Eq. (1.3). Indeed the thermodynamics have been studied by means of the thermodynamic Bethe's ansatz method and a set of two coupled nonlinear integral equations has been derived<sup>39,40</sup> whose solution gives the free energy at all  $T$ . These integral equations have the feature that they do take two distinct forms depending on which of the two regimes  $\Delta$  lies in. In a more picturesque fashion we can say that the integrability of the model extends the low temperature description in terms of particles to all temperatures. For this reason we expect that the dynamics at infinite temperature of the spin-1/2  $XXZ$  model are not generic. The study of the crossover from integrable to generic behavior as next-nearest-neighbor interactions are added would constitute a major step towards formulating what should be called a quantum version of the theorem of Kolmogorov, Arnold, and Moser. Such a theorem would go a long way towards clarifying the status of diffusion at high temperatures in quantum-mechanical systems.

Finally we remind the reader that because of the integrability of the spin-1/2  $XXZ$  chain it is firmly to be expected that the time-dependent correlations studied in this paper can be exactly evaluated. We hope that the numerical results presented here will stimulate the analytic solution of this problem.

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\*Electronic address:

Klaus.Fabricius@theorie.physik.uni-wuppertal.de

<sup>†</sup>Electronic address: mccoy@insti.physics.sunysb.edu

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