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Dynamic spin-pair correlations in a Heisenberg chain at infinite temperature based on an extended short-time expansion

Markus Böhm and Hajo Leschke

Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstrasse 7, W-8520 Erlangen, Germany

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Abstract. Exact coefficients of the short-time expansion of the spin-pair correlations are computed up to order t^{30} in the one-dimensional spin- $\frac{1}{2}$ Heisenberg model with isotropic nearest-neighbour interaction at infinite temperature. The key points of the computational algorithm are sketched. The newly derived coefficients are used to obtain lower and upper bounds on the pair correlations which are graphically indistinguishable up to times nearly twice as large as those up to which previous bounds are reasonably close together. In view of the spin-diffusion hypothesis the spatial spread of the pair correlations is studied as a function of time, but no indication for a diffusive long-time behaviour is found in the extended time region, where the new bounds provide control.

1. Introduction

Considerable attention has been paid to the dynamics of the spin- $\frac{1}{2}$ Heisenberg chain. Of particular interest is the time-dependent spin-pair correlation function, because its Fourier transform is closely related to the spectra of inelastically scattered neutrons and to the width of the spin resonance line in quasi-one-dimensional magnets. For a review see [1].

Even in the limit of infinite temperature an exact solution for the isotropic chain is not known. In this situation there has been much activity [2–5] to obtain the short-time expansion of the pair correlations. This is a useful first step to gain insight into the spin dynamics, as there are powerful methods which are based on the expansion coefficients. However, the evaluation of these coefficients becomes extremely difficult with increasing order due to the exponential growth of computational effort.

In the present paper we have reconsidered this problem and succeeded in computing the exact coefficients for the isotropic spin- $\frac{1}{2}$ chain at infinite temperature up to order t^{30} . In this way we have extended previous results up to t^{16} [3] and confirmed estimates for higher autocorrelation coefficients derived in [5] by finite-chain diagonalizations. The general algorithm and the key points of the computer program are outlined in section 2.

In section 3 we use the newly derived coefficients as a basis to compute lower and upper bounds on the pair correlations by following the method of [6] and its generalization by [2]. In section 4 we propose to test the spin-diffusion hypothesis by bounding the spatial spread of the pair correlations as a function of time.

2. Formulation of the problem and evaluation of expansion coefficients

The Heisenberg chain [7, 8] with isotropic nearest-neighbour interaction and without external magnetic field is specified by the Hamiltonian

$$H := -2J \sum_{n=-N}^N (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z) \quad \text{with } S_{N+1}^\alpha \equiv S_{-N}^\alpha. \quad (1)$$

Here S_n^α denotes the α th component ($\alpha = x, y, z$) of a quantum spin operator located at the n th site of a one-dimensional lattice with unit lattice constant, a total number of $2N + 1$ sites, and cyclic boundary conditions. The macroscopic limit of the normalized time-dependent spin-pair correlation function at infinite temperature T is given as (in units with $\hbar \equiv 1$)

$$C(n, t) := \lim_{N \rightarrow \infty} \frac{\langle S_0^z S_n^z(t) \rangle_{T \rightarrow \infty}}{\langle S_0^z S_0^z \rangle_{T \rightarrow \infty}} = \lim_{N \rightarrow \infty} \frac{\text{Tr}(S_0^z e^{itH} S_n^z e^{-itH})}{\text{Tr}(S_0^z S_0^z)}. \quad (2)$$

This function satisfies

$$|C(n, t)| \leq 1 \quad (3)$$

$$\sum_{n=-\infty}^{\infty} C(n, t) = 1 \quad (4)$$

$$C(n, t) = C(-n, t) = C(n, -t) \quad (5)$$

$$C(n, 0) = \delta_{n0}. \quad (6)$$

The infinite-temperature limit is responsible for the real-valuedness of $C(n, t)$, the symmetry (5), and the triviality of the static correlations (6). The boundedness (3) is a consequence of our normalization. The sum rule (4) follows from the conservation of the total spin

$$\frac{d}{dt} \sum_{n=-N}^N S_n^z(t) = 0 \quad (7)$$

in combination with (6). The symmetry (5) implies that $C(n, t)$ depends only on the absolute value of the (exchange) interaction constant J . Since, in the present paper, we only consider an isotropic interaction, the correlation function does not depend on the particular spin component chosen ($\alpha = z$).

Due to (5) the Taylor expansion of $C(n, t)$ about $t = 0$ can be written as

$$C(n, t) =: \sum_{l=0}^{\infty} \frac{(-1)^l}{(2l)!} M_{2l}(n) (Jt)^{2l}. \quad (8)$$

By expanding the exponentials in (2) the dimensionless coefficients $M_{2l}(n)$ defined through (8) are seen to be expressible as the macroscopic limit of the trace of iterated commutators

$$M_{2l}(n) = \lim_{N \rightarrow \infty} \frac{\text{Tr}(S_0^z \{H^{2l}, S_n^z\})}{J^{2l} \text{Tr}(S_0^z S_0^z)}. \quad (9)$$

Here the m -fold iterated commutator of the Hamiltonian H with an arbitrary operator A on the Hilbert space for the $2N + 1$ spins is denoted by a curly bracket and recursively defined by

$$\{H^0, A\} := A \quad \{H^{m+1}, A\} := H\{H^m, A\} - \{H^m, A\}H. \quad (10)$$

As observed earlier [4], the trace in the nominator of (9) can be evaluated more efficiently by using its cyclic invariance

$$\text{Tr}(S_0^z \{H^{2l}, S_n^z\}) = (-1)^l \text{Tr}(\{H^l, S_0^z\} \{H^l, S_n^z\}). \quad (11)$$

The two commutators on the right-hand side are less iterated and identical apart from a shift by n lattice sites. One should note that $M_{2l}(n)$ vanishes for $l < |n|$ because of $\text{Tr} S_n^\alpha = 0$. Moreover, for the special case of spin- $\frac{1}{2}$ operators

$$S_n^\alpha S_n^\beta = \frac{1}{4} \delta_{\alpha\beta} \mathbf{1} + \frac{i}{2} \sum_\gamma \epsilon_{\alpha\beta\gamma} S_n^\gamma \quad (12)$$

all coefficients $M_{2l}(n)$ are integer valued.

For spin $\frac{1}{2}$ we have computed the pre-limit expression in (9) with exact integer arithmetic for a closed chain consisting of $2N + 1 = 31$ sites thereby getting all non-zero coefficients $M_{2l}(n)$ for the infinite chain corresponding to a short-time expansion up to order t^{30} . In accordance with (11) we had to evaluate commutators up to the 15th iteration. The result for the l -fold commutator $\{H^l, S_n^z\}$ is a sum of products of spin operators corresponding to various components and lattice sites. By using the spin- $\frac{1}{2}$ formula (12) each product can be reduced to a product containing at most one spin operator associated with a given site. The total number of different reduced products increases exponentially with l . For the 15-fold commutator this amounts to a sum of more than 13 million different products. In order to overcome the arising computer storage problem we had to develop a program that makes efficient use of the available storage capacity. The two key points of this program are sketched as follows.

(i) The reduced products are stored in a very compressed form. For each of the 31 sites which underly a given product 2 bit are needed to store one of the four possibilities: S^x, S^y, S^z or $\mathbf{1}$. This implies that each reduced product can be stored in a 64-bit integer. Clearly, since a given reduced product may occur many times in $\{H^l, S_n^z\}$, a combinatorial factor counting the total number of occurrences also has to be stored.

(ii) The $(l + 1)$ -fold commutator $\{H^{l+1}, S_n^z\}$ is evaluated by calculating the one-fold commutator of H with each of the different reduced products occurring in the one-fold commutator $\{H^l, S_n^z\}$, one after the other. In between, the resulting new reduced products are immediately collected into different products with the appropriate combinatorial factors by summing identical products. In doing this the required storage capacity is reduced by a factor of the order of 10 in comparison with the more standard procedure which first calculates $\{H, \{H^l, S_n^z\}\}$ completely and performs the collection afterwards.

By these two points we were able to compute the coefficients $M_{2l}(n)$ up to $2l = 30$ using less than 200 Mbyte of storage capacity. Another advantage of the first point is a saving of computer time, because not only the calculation of the

Table 1. Exact coefficients $M_{2l}(n)$ up to $2l \approx 30$. The coefficients which are not listed are zero.

| | | 2l | | | | | | | | | | |
|----|---|---------------------------|-----|------|--------------------|----------|-----------------------------|----------------------|----------------|--|------------------------|--------------------------------|
| n | 0 | 2 | 4 | 6 | 8 | 10 | 12 | 14 | 16 | | | |
| 0 | 1 | 4 | 44 | 652 | 11 636 | 242 816 | 5 896 200 | 166 988 876 | 5 522 663 076 | | | |
| 1 | | -2 | -28 | -456 | -8 464 | -177 424 | -4 199 416 | -112 473 076 | -3 410 887 248 | | | |
| 2 | | | 6 | 150 | 3 304 | 73 200 | 1 677 302 | 39 475 150 | 908 113 680 | | | |
| 3 | | | | -20 | -728 | -20 292 | -525 316 | -13 331 916 | -335 808 000 | | | |
| 4 | | | | | 70 | 3 360 | 113 454 | 3 369 938 | 94 555 188 | | | |
| 5 | | | | | | -252 | -15 048 | -597 168 | -20 045 896 | | | |
| 6 | | | | | | | 924 | 66 066 | 3 013 868 | | | |
| 7 | | | | | | | | -3 432 | -286 000 | | | |
| 8 | | | | | | | | | 12 870 | | | |
| n | | 18 | | | 20 | | | 22 | | | 24 | |
| 0 | | 212 691 519 520 | | | 9 480 072 152 976 | | | 485 032 014 072 352 | | | 28 212 945 137 704 000 | |
| 1 | | -116 962 174 080 | | | -4 531 208 746 208 | | | -198 947 230 059 248 | | | -9 986 775 178 892 640 | |
| 2 | | 16 874 051 352 | | | -63 733 521 264 | | | -40 087 235 161 232 | | | -3 966 259 880 308 512 | |
| 3 | | -8 316 117 800 | | | -199 629 074 752 | | | -4 998 644 314 328 | | | -206 286 476 494 608 | |
| 4 | | 2 577 229 172 | | | 69 435 334 548 | | | 1 935 670 028 404 | | | 64 615 374 310 856 | |
| 5 | | -618 093 208 | | | -18 156 783 496 | | | -519 107 823 752 | | | -14 753 594 225 776 | |
| 6 | | 112 915 972 | | | 3 801 588 552 | | | 119 956 322 692 | | | 3 629 461 471 962 | |
| 7 | | -14 747 772 | | | -610 327 880 | | | -22 300 656 440 | | | -753 383 387 028 | |
| 8 | | 1 225 224 | | | 70 476 016 | | | 3 193 887 308 | | | 125 955 292 518 | |
| 9 | | -48 620 | | | -5 206 760 | | | -330 540 112 | | | -16 283 892 544 | |
| 10 | | | | | 184 756 | | | 21 985 964 | | | 1 526 926 944 | |
| 11 | | | | | | | | -705 432 | | | -92 357 328 | |
| 12 | | | | | | | | | | | 2 704 156 | |
| n | | 26 | | | | | 28 | | | | | 30 |
| 0 | | 1 845 697 627 092 687 232 | | | | | 134 276 285 717 364 346 136 | | | | | 10 746 808 538 882 581 859 580 |
| 1 | | -580 044 021 167 198 816 | | | | | -39 300 721 390 551 686 224 | | | | | -3 096 927 879 271 998 315 676 |
| 2 | | -326 861 716 633 192 300 | | | | | -25 896 879 848 091 940 506 | | | | | -2 054 656 732 078 694 150 578 |
| 3 | | -18 773 640 799 681 400 | | | | | -2 146 567 001 361 632 748 | | | | | -237 481 854 157 815 112 732 |
| 4 | | 3 163 726 377 228 610 | | | | | 213 322 276 162 807 920 | | | | | 15 307 900 636 441 938 042 |
| 5 | | -418 993 815 097 420 | | | | | -9 508 124 719 510 200 | | | | | 334 414 329 236 534 424 |
| 6 | | 106 047 539 461 210 | | | | | 2 823 714 665 057 340 | | | | | 37 759 472 873 937 630 |
| 7 | | -24 140 280 712 900 | | | | | -743 174 345 775 600 | | | | | -22 046 921 192 632 680 |
| 8 | | 4 540 228 805 200 | | | | | 153 816 389 306 670 | | | | | 4 981 412 562 290 370 |
| 9 | | -689 667 360 660 | | | | | -26 438 166 339 000 | | | | | -944 995 079 449 020 |
| 10 | | 81 261 225 020 | | | | | 3 679 762 140 210 | | | | | 149 551 489 795 710 |
| 11 | | -6 965 727 560 | | | | | -398 298 764 340 | | | | | -19 207 656 508 740 |
| 12 | | 386 308 000 | | | | | 31 444 059 690 | | | | | 1 922 679 759 450 |
| 13 | | -10 400 600 | | | | | -1 610 012 880 | | | | | -140 673 341 520 |
| 14 | | | | | | | 40 116 600 | | | | | 6 689 443 050 |
| 15 | | | | | | | | | | | | -155 117 520 |

commutator of H with a single reduced product can be done with bit manipulation, but also the necessary equality checks during the subsequent collection become faster. As a minor point we want to mention that we had to extend the integer arithmetic, since the higher coefficients do not fit into 64-bit integers.

The final results for the coefficients $M_{2l}(n)$ are presented in table 1. The first

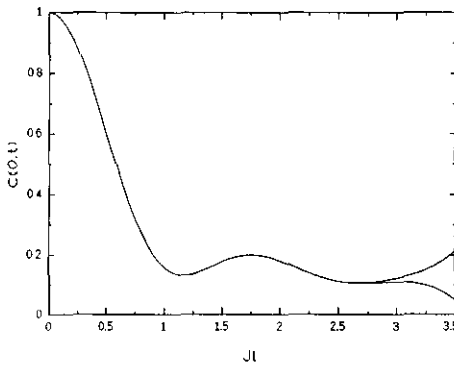


Figure 1. Lower and upper bound on the normalized autocorrelation function $C(0, t)$.

part of the table up to $2l = 16$ is identical to the result of [3] and is given here for completeness. To our knowledge all coefficients corresponding to $2l \geq 18$ are new. Approximate results for the autocorrelation coefficients $M_{2l}(0)$ up to $2l = 30$, which are based on numerical diagonalization of finite chains of up to 11 spins, were reported earlier [5]. The significant digits of these results are now seen to be correct.

3. Bounds on the correlation functions

Since the method of obtaining bounds on correlation functions is well known [2, 4, 6], we sketch only the main points. The temporal Fourier transform of the autocorrelation function

$$\tilde{C}(0, \omega) := \int_{-\infty}^{\infty} \frac{dt}{2\pi} C(0, t) \cos \omega t \tag{13}$$

is an even probability density on the real line of frequencies, that is

$$\tilde{C}(0, -\omega) = \tilde{C}(0, \omega) \geq 0 \quad \int_{-\infty}^{\infty} d\omega \tilde{C}(0, \omega) = 1. \tag{14}$$

The non-negativity of $\tilde{C}(0, \omega)$ follows from that of the dynamic structure factor. In consequence, the autocorrelation coefficients $M_{2l}(0)$ are not only generated by a Taylor expansion but also related to the even moments of a probability density

$$\int_{-\infty}^{\infty} d\omega \tilde{C}(0, \omega) \omega^{2l} = J^{2l} M_{2l}(0). \tag{15}$$

The equation for the inverse transformation

$$C(0, t) = \int_{-\infty}^{\infty} d\omega \tilde{C}(0, \omega) \cos \omega t \tag{16}$$

therefore suggests the following procedure to compute a lower (respectively upper) bound on $C(0, t)$. Within the set of all even probability densities with prescribed even moments $J^{2l} M_{2l}(0)$ ($l = 0, \dots, l_{\max}$) one has to determine—at the given time t —a density which gives the smallest (respectively largest) average of $\cos \omega t$. As an extremizing density one can always take a suitably weighted sum of $l_{\max} + 1$ Dirac delta-functions located at suitable frequencies. In practice, the frequencies and weights can be found numerically by a linear-programming method [6].

The results of our computations with $l_{\max} = 15$ are plotted in figure 1. On the given scale the lower and the upper bound on $C(0, t)$ are graphically indistinguishable up to times $Jt = 2.8$. We have confirmed previous observations [4, 6] that, over the time interval considered, the lower (respectively upper) bound agrees excellently with the so-called principal representation [9] which uses at all times the frequencies and weights of the Gaussian quadrature formula corresponding to the given finite set of $l_{\max} = 15$ (respectively $l_{\max} = 14$) moments. Therefore, the principal representation appears to be well suited to provide fairly reliable results rapidly. The simplest approach to $C(0, t)$ is a truncation of the Taylor series (8). Such a truncation also leads to bounds on $C(0, t)$, because the cosine function is bounded by its truncated power series alternately from below and above. However, the bounds obtained in this way are graphically indistinguishable only up to times $Jt = 1.8$ and diverge rapidly for larger times.

We have tried out the maximum-entropy method (see, for example, [10]) to obtain a so-called unbiased extrapolation of $C(0, t)$ to times $Jt > 2.8$. However, we did not succeed in handling the serious convergence problems related to the relatively large number of prescribed moments. In any case, figure 1 clearly shows that the results for $C(0, t)$ presented in figure 3(b) of [10] are less reliable than claimed by the authors. This supports our belief that the power of the maximum-entropy method is often overestimated.

Obtaining bounds on the correlation function of two spins at different sites is not this straightforward, because the temporal Fourier transform of $C(n, t)$ with $n \neq 0$ has no unique sign. Therefore, we first consider the spatial Fourier transform of the pair correlation

$$I(k, t) := \sum_{n=-\infty}^{\infty} C(n, t) \cos kn \quad |k| \leq \pi \quad (17)$$

which is sometimes also called the intermediate structure factor. The following properties of $I(k, t)$ are simple consequences of (4)–(6)

$$I(k, t) = I(-k, t) = I(k, -t) \quad (18)$$

$$I(0, t) = I(k, 0) = 1. \quad (19)$$

As the short-time expansion coefficients of $I(k, t)$ are simply the spatial Fourier transform of those of $C(n, t)$ and the temporal Fourier transform of $I(k, t)$ is the non-negative dynamic structure factor, one can compute bounds on $I(k, t)$ —for given wavenumber k —analogously to those on $C(0, t)$. For example, the inequalities $|\cos \omega t| \leq 1$ and $1 - \frac{1}{2}(\omega t)^2 \leq \cos \omega t$ immediately imply

$$|I(k, t)| \leq 1 \quad (20)$$

and

$$1 - 2(1 - \cos k)(Jt)^2 \leq I(k, t). \quad (21)$$

But again one can do better numerically by applying the procedure of [6] (see [4]). By using all coefficients of table 1 we thus have obtained bounds which are plotted in

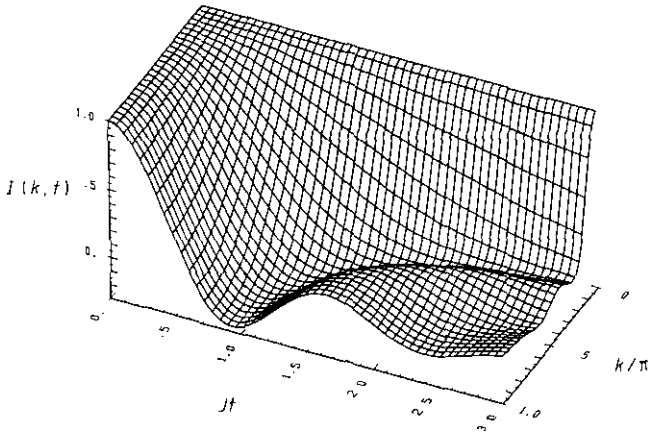


Figure 2. Arithmetic mean of the lower and upper bound on the intermediate structure factor $I(k, t)$.

figure 2. Again, these bounds are graphically indistinguishable up to times $Jt = 2.8$. One should note that $I(k, t)$ exhibits oscillations and has no unique sign.

Following [2], the bounds on $I(k, t)$ can now be used to obtain bounds on $C(n, t)$ by performing the inverse transformation

$$C(n, t) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} I(k, t) \cos kn \tag{22}$$

piecewise. More precisely, by using for the (numerical) integration over k the lower (respectively upper) bound on $I(k, t)$ if $\cos kn$ is positive (respectively negative) and the upper bound on $I(k, t)$ if $\cos kn$ is negative (respectively positive), one gets a lower (respectively upper) bound on $C(n, t)$.

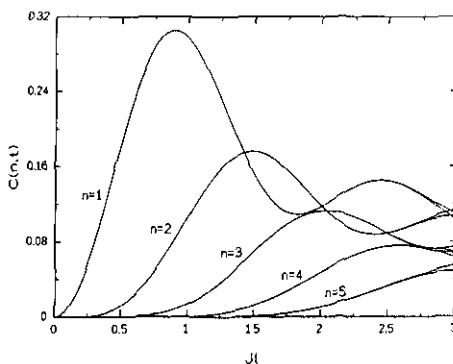


Figure 3. Lower and upper bound on the normalized correlation function $C(n, t)$ for the near neighbours $n = 1, \dots, 5$.

The final results are plotted in figure 3. Corresponding lower and upper bounds on the near-neighbour correlations are graphically indistinguishable up to times $Jt = 2.7$. The previous bounds in [2] are indistinguishable only up to $Jt = 1.6$. From figures 1 and 3 it is seen that in the time region accessible to our bounds the

correlation functions $C(n, t)$ for $n = 0, 1, \dots, 5$ are still oscillating but remain positive.

4. Bounds on the spatial variance and the diffusion hypothesis

For the isotropic Heisenberg model and for more general spin models for which one component of the total spin is conserved (7), it is often claimed that the high-temperature spin dynamics on large time and space scales can be described by a diffusion process (see, for example, [1]). In this context the isotropic spin- $\frac{1}{2}$ Heisenberg chain is of particular interest, because for this model the validity of the diffusion hypothesis is least clear for two reasons.

(i) A general observation is that the correlation functions oscillate the more strongly the smaller the spin quantum number and space dimension are.

(ii) For the isotropic spin- $\frac{1}{2}$ XY chain (dropping $S_n^z S_{n+1}^z$ in (1)) it is known [11, 12] that no diffusion emerges asymptotically, although (7) remains true.

Our concern in this section is to see whether the spin-diffusion picture is supported by the extended short-time expansion.

Even though we extended the time region to where the bounds on the individual correlation functions $C(n, t)$ are reasonably close together, the remaining oscillations did not allow us to decide for or against a diffusive leading $t^{-1/2}$ behaviour for large t . Nor does the time dependence of $I(k, t)$ for small k develop the diffusive exponential decay in the time region accessible to us. As an alternative way to proceed we propose looking at the quantity

$$\sigma^2(t) := \sum_{n=-\infty}^{\infty} C(n, t)n^2 \quad (23)$$

which we call the spatial variance of the pair correlation function, although we do not strictly know whether $C(n, t)$ remains non-negative for all t . Nevertheless, we believe that it is a natural measure for the spread of the 'spin density' and hence a quantity more adapted to testing the diffusion hypothesis. In the diffusive case its leading behaviour for large t should be linear, that is

$$\sigma^2(t) \sim 2Dt \quad (24)$$

where D denotes the diffusion constant.

We note that $\sigma^2(t)$ equals—up to a sign—the second derivative of $I(k, t)$ with respect to k at $k = 0$. This relation can be written as

$$\sigma^2(t) = 2 \lim_{k \rightarrow 0} \frac{1 - I(k, t)}{k^2} \quad (25)$$

according to (18) and (19). By this equation bounds on $I(k, t)$ induce bounds on $\sigma^2(t)$. For example, inequalities (20) and (21) immediately imply

$$0 \leq \sigma^2(t) \leq 2(Jt)^2. \quad (26)$$

Of course, sharper bounds on $\sigma^2(t)$ can be computed numerically by using in (25) the bounds underlying figure 2. Our results for these bounds are plotted in figure 4.

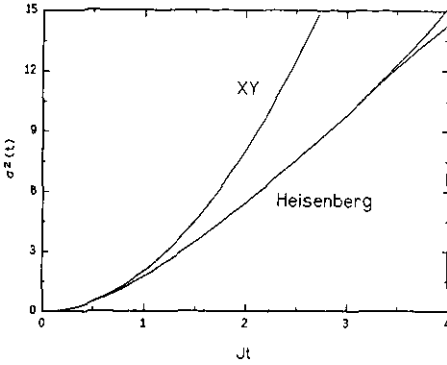


Figure 4. Lower and upper bound on the spatial variance $\sigma^2(t)$ of the Heisenberg chain (lower curves) and the exact spatial variance $\sigma_{XY}^2(t)$ of the XY chain (upper curve).

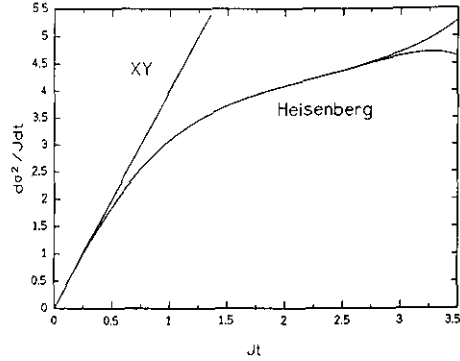


Figure 5. Lower and upper bound on the time derivative of the spatial variance $d\sigma^2(t)/dt$ (lower curves) and the time derivative of the spatial variance $d\sigma_{XY}^2(t)/dt$ (upper curve).

The bounds are graphically indistinguishable up to times $Jt = 3.3$. In contrast to other quantities the spatial variance seems to reveal no oscillations thereby supporting our belief that it is a more appropriate quantity for testing the diffusion hypothesis.

In order to see more clearly whether there is any indication for a diffusive long-time behaviour of $\sigma^2(t)$, we have numerically computed bounds on its time derivative $d\sigma^2(t)/dt$. This can be done by starting from the time derivative of (25). The required bounds on $\partial I(k, t)/\partial t$ can be obtained by substituting $-\omega \sin \omega t$ for $\cos \omega t$ in the linear-programming procedure. The lower and upper bound on $d\sigma^2(t)/dt$ are plotted in figure 5. For this derivative we observe a linear behaviour with slope $4J^2$ up to times $Jt \approx 0.3$. After a cross-over regime another linear behaviour with slope $\approx 0.6J^2$ emerges about $Jt = 1.7$. The behaviour beyond $Jt = 2.7$ is not accessible to our bounds.

On the basis of these findings we see essentially two distinct possibilities for the long-time behaviour:

(i) The asymptotic regime is reached already for $Jt \geq 1.7$. This would imply a non-diffusive long-time behaviour of the form

$$\sigma^2(t) \sim A(Jt)^2 \quad A \approx 0.3 \tag{27}$$

(ii) There is another cross-over beyond $Jt = 2.7$ to a diffusive long-time behaviour of the form (24) with

$$D \geq 2.3J. \tag{28}$$

There will have to be further investigations to reach a decision between these two alternatives.

For the purpose of comparison it is instructive to calculate the spatial variance $\sigma_{XY}^2(t)$ for the isotropic spin- $\frac{1}{2}$ XY chain by using the exact result of [11] (see also [12]) for the longitudinal pair correlations. By substituting for $C(n, t)$ in (23) the squared Bessel functions we find (see formula (5.7.12.21) of [13])

$$\sigma_{XY}^2(t) = \sum_{n=-\infty}^{\infty} [J_n(2Jt)]^2 n^2 = 2(Jt)^2. \tag{29}$$

This result reflects the well-known non-diffusive behaviour and coincides with the upper bound in (26). It is also shown in figures 4 and 5. As is suggested by figure 5, the second inequality in (26) still holds after differentiation with respect to t .

Some readers might wish to compare our findings with results for the corresponding classical spin chains. Here computer-simulation methods [14, 15] allow one to obtain data for the time-dependent pair correlations in chains of up to 20 000 spins which are believed to be statistically significant for times as large as $Jt = 100$ [15]. These data convincingly suggest the existence of a $t^{-\alpha}$ long-time tail, although there has been a debate [16] on the question whether the value of the exponent α is strictly $\frac{1}{2}$ or not. While these results for classical chains are of much interest in their own right, the reader should resist the temptation to draw conclusions from them about chains in the extreme quantum limit of spin $\frac{1}{2}$. She or he only needs to realize that in [15] a diffusive long-time behaviour is convincingly suggested not only for the classical Heisenberg chain but also for the classical XY chain.

5. Conclusion and outlook

The coefficients of the short-time expansion of the spin-pair correlations have been evaluated up to order t^{30} for the isotropic spin- $\frac{1}{2}$ Heisenberg chain at infinite temperature. Using these coefficients we improved previous bounds on the autocorrelation as well as on the near-neighbour correlations. In the extended time region, where the bounds are reasonably close together, the correlation functions do still oscillate and remain positive. Both facts are not understood analytically. Although we supplied some control for the time dependence of the spatial spread of the pair correlations, the validity of the spin-diffusion hypothesis remains open.

With the improved algorithm we also have computed the coefficients up to order t^{28} for anisotropic XYZ chains thereby extending the work of [4] and [2], who gave these more general coefficients corresponding to t^{10} and t^{14} respectively. Our result is too long to be printed here. However, in a forthcoming publication we plan to present selected results on anisotropic chains which may be compared with experimental data for quasi-one-dimensional magnets.

Acknowledgment

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References

- [1] Steiner M, Villain J and Windsor C G 1976 *Adv. Phys.* **25** 87
- [2] Brandt U and Stolze J 1986 *Z. Phys. B* **64** 327
- [3] Nagao N and Miyagi H 1976 *Prog. Theor. Phys.* **55** 21
- [4] Roldan J M R, McCoy B M and Perk J H H 1986 *Physica* **136A** 255
- [5] Sur A and Lowe I J 1975 *Phys. Rev. B* **11** 1980
- [6] Platz O and Gordon R G 1973 *Phys. Rev. Lett.* **30** 264; 1973 *Phys. Rev. B* **7** 4764
- [7] Heisenberg W 1928 *Z. Phys.* **49** 619
- [8] Mattis D C 1988 *The Theory of Magnetism I* (Berlin: Springer)
- [9] Gordon R G 1968 *J. Math. Phys.* **9** 655
- [10] Mead L R and Papanicolaou N 1984 *J. Math. Phys.* **25** 2404

- [11] Niemeijer T 1967 *Physica* **36** 377
- [12] Katsura S, Horiguchi T and Suzuki M 1970 *Physica* **46** 67
- [13] Prudnikov A P, Brychkov Yu A and Marichev O I 1988 *Integrals and Series* vol 2 (New York: Gordon and Breach)
- [14] Müller G 1988 *Phys. Rev. Lett.* **60** 2785
- [15] Gerling R W and Landau D P 1990 *Phys. Rev. B* **42** 8214
- [16] Gerling R W and Landau D P 1989 *Phys. Rev. Lett.* **63** 812
- Müller G 1989 *Phys. Rev. Lett.* **63** 813