Dynamics of the classical planar spin chain

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In this paper we pay attention to the classical one-dimensional planar spin system and, in particular, to the dynamics of such a model. We use the Monte Carlo method to calculate the static correlation functions, needed to determine the relaxation functions completely. We are then able to give the results for the in- and out-of-plane component of the relaxation function. At low temperatures the excitations of the out-of-plane component behave as free particles while the excitations of the in-plane component are very similar to the excitations in the Heisenberg chain.

I. INTRODUCTION

The dynamics of one-dimensional magnetic systems is very interesting because well-defined spin-wave excitations are observed[1-4] at nonzero temperatures although there is no magnetization.[5]

A spin chain is called planar if an anisotropic term is added to the Heisenberg exchange interaction such that the spins are forced in the x-y plane. The substance $CsNiF_3$ is well described by the model as was shown by a lot of static and dynamic measurements.[4] The material is a spin-one system which means that quantum-mechanical effects play an important role. A transformation to semipolar coordinates, as proposed by Villain,[6] made it possible to calculate low-temperatures properties for the quantum system.[6,7]

For the classical planar chain, it is not possible to calculate all static quantities analytically as is the case for the classical Heisenberg chain.[8,9] It is possible to calculate several interesting static quantities by means of the transfer-operator method.[10]

Loveluck and Lovesey also obtained results for the out-of-plane component of the relaxation function[11] by expressing the moments of the relaxation function in terms of spin-correlation functions which could be calculated numerically. It is practically impossible to calculate the in-plane component of the relaxation function or to obtain better approximations for the relaxation function in this way because of the amount of work which is necessary to evaluate the correlation functions.

In this paper, we will shown that the Monte Carlo method[12] is very useful to calculate correlation functions of time derivatives without the need of analytic expressions in terms of static spin-correlation functions. It will be obvious that this method can be applied to other models as well.

In Sec. II we derive the relaxation function using Mori's formalism[13-15] and we calculate the frequency-dependent transport coefficients with the method given in our earlier paper.[15] In Sec. III we discuss the various possibilities to calculate the static quantities appearing in our relaxation function and we compare our results with results obtained by other methods. In Sec. IV we give extensive numerical results. We also calculate the dynamic form factor as a function of temperature for the in-plane and out-of-plane component.

II. DYNAMIC EQUATIONS

A planar spin chain, with nearest-neighbor interaction J, is described by the Hamiltonian[4]

$$H = -J \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + A \sum_n (S_n^z)^2 . \tag{2.1}$$

If the anisotropy A is positive, the spins will be forced in the x-y plane as the temperature decreases. When A is negative, the spins will prefer to stand along the z axis. It is convenient to introduce Fourier transformed operators by

$$\vec{S}_k = \frac{1}{\sqrt{N}} \sum_n e^{ikn} \vec{S}_n . \tag{2.2}$$

and then the Hamiltonian reads

$$H = -J \sum_k \vec{S}_k \cdot \vec{S}_{-k} \cos k + A \sum_k S_k^z S_{-k}^z . \tag{2.3}$$

In the following, we will only be concerned with the classical model for which one is able to calculate certain static correlation functions.[10] In a classical model, the spins are replaced by angular momenta of unit length that can stand in any direction.

If we want to study the dynamics of this system, we have to calculate the time-dependent spin-spin correlation functions. These functions can be measured directly by inelastic neutron scattering.[4]

We will use the Mori projection operator formalism[13-15] and therefore we have to find the quantities that describe the slow motion of the system in order to separate these modes from modes that decay fast in time.

Because we have a classical system, we define the scalar product as the static susceptibility

$$(S^a, S^a)_k = \beta \langle S_k^a S_{-k}^a \rangle, \quad a = x, y, z . \tag{2.4}$$

As usual, β denotes the inverse temperature (we use units such that $\hbar = 1$, $k_B = 1$). The Liouville operator L determines the time evolution

$$S_k^a(t) = e^{iLt} S_k^a(0) , \tag{2.5}$$

and is related to the Hamiltonian by

$$L S_k^a = [H, S_k^a] , \tag{2.6}$$

where the square brackets denote the Poisson brackets. Then the Laplace transform of the time-dependent relaxation function can be written[16]

$$\Phi_{SS}^{ab}(z, k) = (S^a, (z - L)^{-1} S^b)_k$$
$$= -i \int_0^\infty dt \, e^{izt} (S^a(t), S^b(0))_k , \tag{2.7}$$

with $z = \omega + i\epsilon$, $\epsilon > 0$.

By symmetry, we have

$$(S^a, (z - L)^{-1} S^b)_k = \delta_{ab} (S^a, (z - L)^{-1} S^a)_k . \tag{2.8}$$

This means that there is no coupling between the different spin components in the dynamic equations. Because the total spin in the z direction is a conserved quantity, we know that S_k^z and its time derivatives $L S_k^z$ and $L^2 S_k^z$ are slow variables. The total spin in the x or y direction is not conserved, but for $A > 0$ it is a critical variable which means that S_k^x and S_k^y are also slow variables.[17]

We do not have such a plausible argument for the time derivatives of S_k^x or S_k^y but as we want to treat S_k^x or S_k^y on the same footing as S_k^z, we will take $L S_k^x$ and $L^2 S_k^x$ as additional variables. Because of Eq. (2.8) we will now ommit the index referring to the spin component since it simplifies the notation considerably. Then we take

$$\left\{ S_k, L S_k, A_k = L^2 S_k - \frac{(LS, LS)_k}{(S, S)_k} \right\} \tag{2.9}$$

as our set of relevant variables. We have replaced the second time derivative $L^2 S_k$ by A_k because the matrix of static susceptibilities

$$\tilde{\chi}_k = \begin{bmatrix} (S, S)_k & 0 & 0 \\ 0 & (LS, LS)_k & 0 \\ 0 & 0 & (A, A)_k \end{bmatrix} \tag{2.10}$$

is diagonal.

The frequency matrix yields

$$\tilde{\Omega}_k = \begin{bmatrix} 0 & 1 & 0 \\ \dfrac{(LS, LS)_k}{(S, S)_k} & 0 & 1 \\ 0 & \dfrac{(A, A)_k}{(LS, LS)_k} & 0 \end{bmatrix} \tag{2.11}$$

and the projector on the subspace spanned by the relevant variables is given by

$$PB_k = \frac{(S, B)_k}{(S, S)_k} S_k + \frac{(LS, B)_k}{(LS, LS)_k} L S_k + \frac{(A, B)_k}{(A, A)_k} A_k , \tag{2.12}$$

where B_k denotes an arbitrary operator.

The projector on the orthogonal complement is $Q \equiv 1 - P$ and because $Q L S_k = Q L^2 S_k = 0$ by construction, the transport matrix contains only one non-zero element

$$\tilde{\Sigma}(z, k) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Sigma_k(z) \end{bmatrix} , \tag{2.13}$$

with

$$\Sigma_k(z) = -(A, A)_k^{-1} (QLA, (z - QLQ)^{-1} QLA)_k . \tag{2.14}$$

The matrix of the relaxation functions

$$\tilde{\Phi}(z, k) \equiv \begin{bmatrix} \Phi_{SS} & \Phi_{SLS} & \Phi_{SA} \\ \Phi_{LSS} & \Phi_{LSLS} & \Phi_{LSA} \\ \Phi_{AS} & \Phi_{ALS} & \Phi_{AA} \end{bmatrix} \tag{2.15}$$

is the solution of the matrix equation

$$[z \tilde{1} - \tilde{\Omega}_k + \tilde{\Sigma}(z, k)] \tilde{\Phi}(z, k) = \tilde{\chi}_k \tag{2.16}$$

and we obtain

$$\Phi_{SS}(z, k) = (S, S)_k \frac{z^2 + z \Sigma_k(z) - (A, A)_k / (LS, LS)_k}{z[z^2 - (L^2 S, L^2 S)_k / (LS, LS)_k] + \Sigma_k(z)[z^2 - (LS, LS)_k / (S, S)_k]} \tag{2.17}$$

for the Laplace transformed spin-spin relaxation function. The imaginary part $\Phi_{SS}''(z,k)$ of this function is related to the dynamic form factor by

$$S(k,\omega) = [-\omega/(1 - e^{-\beta\omega})]\Phi_{SS}''(\omega,k). \qquad (2.18)$$

Until now, no approximations have been made, but Eq. (2.17) still contains the unknown function $\Sigma_k(z)$. If we note the similarity between the formal expression for $\Sigma_k(z)$, given by Eq.(2.14), and Eq. (2.7) we might wonder what we have gained by the formal manipulations that led to Eq. (2.17). The main advantage of this method is the fact that we have made a separation between important contributions to the long-time behavior of the relaxation function and fast fluctuating terms by introducing the projection operator P. At extremely low temperatures, the number of slow modes is large and therefore we can expect that we have to extend our set of variables to have a reasonable description, but this is no principal difficulty. Therefore, the only remaining problem for our dynamic description is to express the transport coefficient $\Sigma_k(z)$ as a function of the frequency and some static susceptibilities.

We derive the equation of motion for the transport coefficient by twice applying the identity[15]

$$z(z - QLQ)^{-1} = 1 + QLQ(z - QLQ)^{-1}, \qquad (2.19)$$

and we find

$$\left(z^2 + \frac{(LA, LA)_k}{(A,A)_k}\right)(QLA, (z - QLQ)^{-1}QLA)_k$$
$$= z(QLA, LA)_k + (QL^3A, (z - QLQ)^{-1}QLA)_k. \qquad (2.20)$$

Now we assume that the last term of the right-hand side of Eq. (2.20) can be replaced by its value for $\omega = 0$. This is a reasonable assumption because this term contains higher time derivatives than all the other terms and we have

$$\left(z^2 + \frac{(LA, LA)_k}{(A,A)_k}\right)(QLA, (z - QLQ)^{-1}QLA)_k$$
$$= z(QLA, LA)_k + \frac{(LA, LA)_k}{(A,A)_k}$$
$$\times (QLA, (i\epsilon - QLQ)^{-1}QLA)_k. \qquad (2.21)$$

Using $(A, B)_k = (B^\dagger, A^\dagger)_{-k}$ and space-reversal invariance, we conclude that the last term of the right-hand side of Eq. (2.21) is purely imaginary and we calculate this term by using the sum rule

$$(QLA, LA)_k = -\frac{1}{\pi}\lim_{\epsilon\to 0}$$
$$\times \int_{-\infty}^{+\infty} d\omega \, \mathrm{Im}(QLA, (z - QLQ)^{-1}QLA)_k. \qquad (2.22)$$

The final expression for the transport coefficient reads

$$\Sigma_k(z) = -\frac{(QLA, LA)_k}{(A,A)_k}$$
$$\times \frac{1}{z + i(LA, LA)_k^{1/2}/(A,A)_k^{1/2}}. \qquad (2.23)$$

It is convenient to express the susceptibilities appearing in this formula in terms of spin-spin susceptibilities and we find

$$(A, A)_k = (L^2S, L^2S)_k - (LS, LS)_k^2/(S, S)_k, \qquad (2.24a)$$

$$(LA, LA)_k = (L^3S, L^3S)_k$$
$$- \frac{2(LS, LS)_k(L^2S, L^2S)_k}{(S,S)_k} + \frac{(LS, LS)_k^3}{(S,S)_k^2}, \qquad (2.24b)$$

$$(QLA, LA)_k = (L^3S, L^3S)_k - \frac{(L^2S, L^2S)_k^2}{(LS, LS)_k}. \qquad (2.24c)$$

Inserting Eq. (2.24) in Eq. (2.17) and expanding the relaxation function for large z values, we obtain

$$\Phi_{SS}(z,k) = \frac{(S,S)_k}{z} + \frac{(LS, LS)_k}{z^3}$$
$$+ \frac{(L^2S, L^2S)_k}{z^5} + \frac{(L^3S, L^3S)_k}{z^7} + \cdots, \qquad (2.25)$$

which means that our relaxation function satisfies the sum rules

$$(L^nS, L^nS)_k = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega \, \omega^{2n}\Phi_{SS}''(\omega, k) \qquad (2.26)$$

for $n = 0, 1, 2$, which is a consequence of the choice of the variables, and for $n = 3$ which shows that our calculation of the transport coefficient is as consistent as possible.

III. STATIC SUSCEPTIBILITIES

In the previous sections, we calculated the Laplace transformed relaxation function as a function of the frequency and the static susceptibilities. In this section, we will discuss the various possibilities to calculate these static quantities.

First of all, it is worthwhile to examine the kind of correlation functions that have to be calculated. Of course, we need all spin-spin correlation functions

$$\langle S_0^a S_n^a\rangle, \quad n = 0, \cdots, N; \quad a = x, y, z \qquad (3.1)$$

in order to calculate the Fourier transformed correlation functions $\langle S_k^a S_{-k}^a\rangle$.

For the susceptibilities of the type (B, LC) the situation is different because the relation

$$(B, LC) = \langle [B^\dagger, C]\rangle \qquad (3.2)$$

can be used to show that in the case of nearest-neighbor interaction

$$(L^j S_0^a, L^j S_n^a) = 0 \quad \text{if } n \geq 2j;$$

$$j = 1, 2, \cdots; \quad a = x, y, z . \quad (3.3)$$

This result reduces the number of terms considerably. However, it turns out that even then, it is a very tedious job to express $(L^j S_0^a, L^j S_n^a)$ in terms of $2j$-spin correlation functions and although an exact expression for $j = 3$ is available for the Heisenberg magnet,[9] it is not surprising that no similar result for the planar chain exists.

Let us now look at the different methods. The very elegant and numerically exact transfer operator method which has been used for the planar chain by Loveluck, Lovesey, and Aubry[10] reduces the problem of calculating the partition function to an eigenvalue problem. Once the eigenvalue problem is solved, one can calculate two-spin, four-spin, and six-spin correlation functions; but as already mentioned, some expressions for the relaxation function are very complicated combinations of the static correlation functions. One could argue that the work done in obtaining such expressions is largely compensated by the fact that one obtains exact results, but if one considers the amount of work and if one realizes that these expressions are only useful for a very small class of Hamiltonians (in our case, the corresponding expressions for the Heisenberg chain should be found by putting $A = 0$), one should conclude to look for other possibilities. Clearly, a more direct and general way to calculate static susceptibilities for classical systems is desirable.

A very general method to study various aspects of classical many-body systems is given by the Monte Carlo method.[12] The initial idea is to write a computer program which simulates the physical system that one would like to study. We do not want to discuss the general aspects of this technique here and therefore only a brief description of the computer program for our spin model will be given.

The first step is to set up the initial spin configuration, for instance a random configuration. Then a spin is selected using a random number and the direction of the selected spin is changed according to three random numbers. The corresponding energy difference ΔE is calculated and if $\exp(-\beta \Delta E) \geq x$ ($0 \leq x \leq 1$, random number) the old spin direction is replaced by the new one. Repeating this procedure M times, one can show that the configurations are distributed according to the canonical ensemble if $M \rightarrow \infty$. Once the system is close enough to its equilibrium, averages of spin combinations are easily calculated.

The disadvantageous aspects of the transfer operator method are not present in this approach. Indeed, we only have to calculate LS_i^a, $a = x, y, z$ and once these expressions have been programmed, the computer takes care of the remaining calculations. Although the program is rather simple, a complete check on the results should be possible to have an idea of the statistical errors which are unavoidable in Monte Carlo calculations. In our case, this is easy because analytic results of the classical Heisenberg model are known. There is an excellent agreement between our numerical values and the exact results. A comparison between some exact results[10] obtained by the transfer operator method and Monte Carlo results for the planar chain is summarized in Table I.

We conclude this section with some general remarks. One might wonder why, since we are doing Monte Carlo after all, we did not use the equations of motions directly in order to obtain the dynamic form factor. Then we should not need the moments explicitly.

The objection to this point is that the integration of the equations of motion is only valid for relatively short times[4] (high frequency) whereas we are interested in spin waves, which are low-frequency (long-time) phenomena. Because the low-frequency region is well described by Mori's formalism, it is an appropriate tool to study these excitations, and therefore a calculation of the moments is necessary. An alternative way to calculate the moments is to calculate the time-dependent correlation functions for short times and because

$$\beta \langle S_i^a(t) S_j^a(0) \rangle = (S_i^a, S_j^a)$$

$$- \frac{t^2}{2!} (LS_i^a, LS_j^a) + \frac{t^4}{4!} (L^2 S_i^a, L^2 S_j^a)$$

$$- \frac{t^6}{6!} (L^3 S_i^a, L^3 S_j^a) + \cdots , \quad (3.4)$$

we can, in principle, obtain numerical values for the moments by calculating the time derivatives of the correlation function. However, it is well

TABLE I. Comparison between exact and Monte Carlo results for $\beta J S^2 = 15$ and $A = 0.21 J$.

Correlation function	Exact	Monte Carlo
$\langle S_0^x S_0^x \rangle / S^2$	0.4751	0.4743
$\langle S_0^x S_2^x \rangle / S^2$	0.4411	0.4365
$\langle S_0^z S_0^z \rangle / S^2$	0.0499	0.0514
$\langle S_0^z S_2^z \rangle / S^2$	0.0147	0.0157

known that, even in very simple cases, this is often one of the hardest problems in numerical calculations. Since we compute static susceptibilities appearing in Eq. (3.4) directly, we can compare the time-dependent correlation function with the values obtained by integrating the equations of motion, and for short times there is an excellent agreement. This supports the fact that the calculation of the moments from the data obtained by integrating the equations of motion is a very difficult numerical problem.

IV. DISCUSSION OF THE RESULTS

As said in Sec. III, the quantities that are calculated are two site correlation functions of the spins and their derivatives. These have to be multiplied with the inverse temperature to yield the corresponding susceptibilities. We always took $A = 0.21J$, because this value corresponds to the anisotropy in $CsNiF_3$, for which measurements are available.

In Fig. 1 we give the self correlation function and the correlation function between nearest neighbors, for the x and z components and the exact results for the Heisenberg chain $(A = 0)$. From these results we obtain

$$(LS^z, LS^z)_k = 4J(1 - \cos k)\langle S_0^x S_1^x \rangle, \qquad (4.1)$$

$$(LS^x, LS^x)_k = 2A[\langle (S_0^x)^2 \rangle - \langle (S_0^z)^2 \rangle]$$
$$+ 2J(1 - \cos k)(\langle S_0^x S_1^x \rangle + \langle S_0^z S_1^z \rangle). \quad (4.2)$$

In Figs. 2–7 results for some correlation functions of time derivatives are shown. To find the k-de-

pendent susceptibilities we perform a Fourier transformation and using Eq. (3.3) we find

$$(L^j S^a, L^j S^a)_k = (L^j S_0^a, L^j S_0^a)$$
$$+ 2 \sum_{n=1}^{2j-1} \cos(kn)(L^j S_0^a, L^j S_n^a). \quad (4.3)$$

The most difficult quantity to extract from the

FIG. 2. Self-correlation function of the second time derivative of a spin component. To get the corresponding susceptibility, one must multiply with $\beta J^4 S^6$. The meaning of the x, z, and H symbols is the same as in Fig. 1.
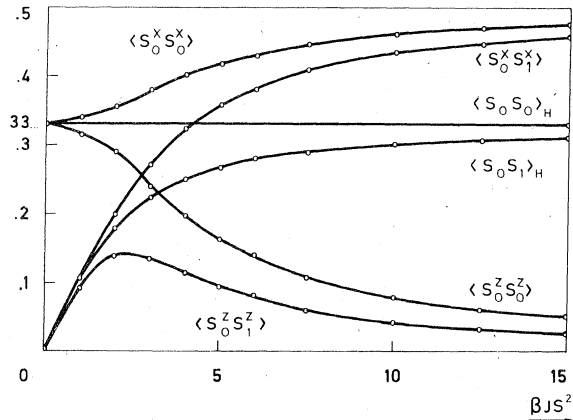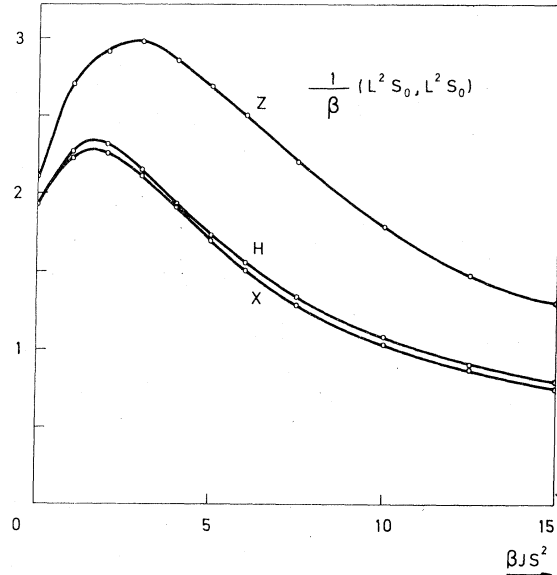

FIG. 1. Self-correlation function and the nearest-neighbor correlation function as a function of $\beta J S^2$, where β is the inverse temperature. The in-plane, out-of-plane, and Heisenberg results are marked by x, z, and H, respectively. The correlation functions are given in units of S^2.
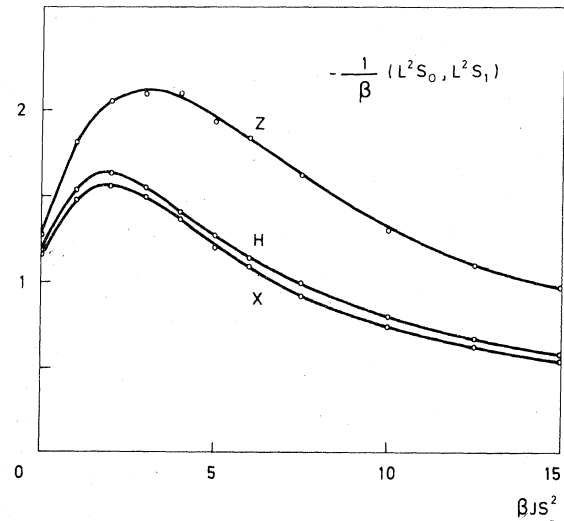

FIG. 3. Correlation function between the second time derivatives of nearest neighbors. See also Fig. 2.

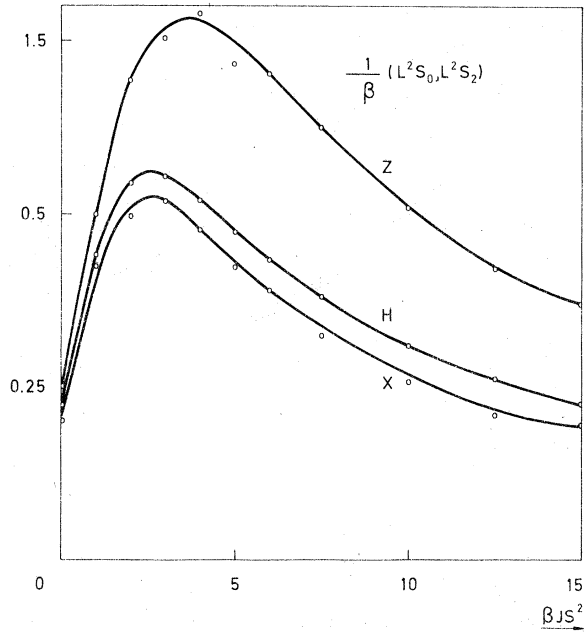FIG. 4. Correlation function between the second time derivatives of next-nearest neighbors. See also Fig. 2.

FIG. 6. Correlation function between the third time derivatives of nearest neighbors. See also Fig. 5.

numerical results is the wave-vector-dependent correlation function, because at finite temperatures all $\langle S_0^a S_n^a \rangle$ are different from zero, and consequently contribute to $\langle S_k^a S_{-k}^a \rangle$. From results ob-
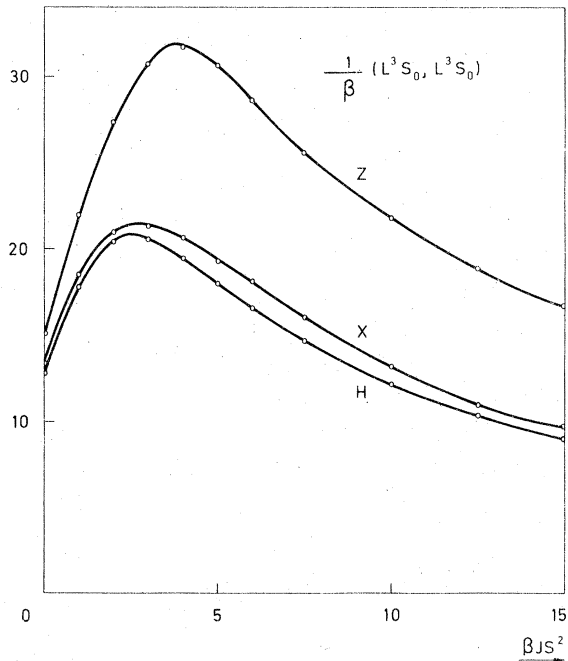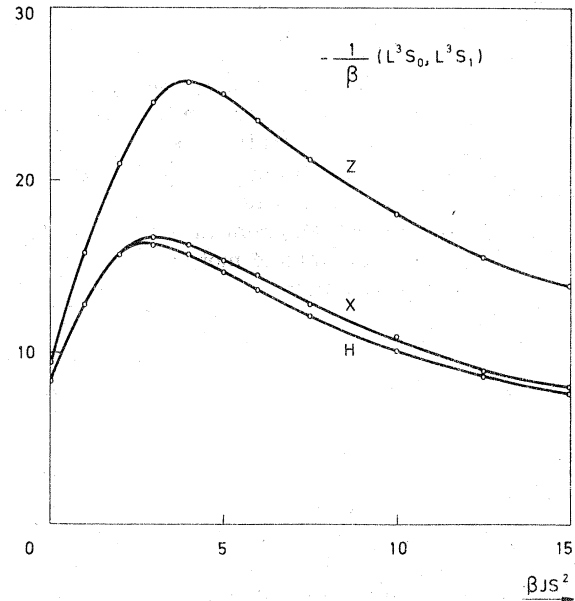
tained by Loveluck, Lovesey, and Aubry[10] for the planar chain, and knowing the exact result for the Heisenberg chain

$$\langle S_0^x S_n^x \rangle = \langle S_0^y S_n^y \rangle = \langle S_0^z S_n^z \rangle = \tfrac{1}{3} S^2 e^{-\kappa_H^{(\beta)n}}, \qquad (4.4)$$

it seems justified to suppose the following behavior:

$$\langle S_0^a S_n^a \rangle = \langle (S_n^a)^2 \rangle e^{-\kappa_a^{(\beta)n}}; \quad a = x, y, z \qquad (4.5)$$

FIG. 5. Self-correlation function of the third time derivative of a spin component. To get the corresponding susceptibility one must multiply with $\beta J^6 S^8$.
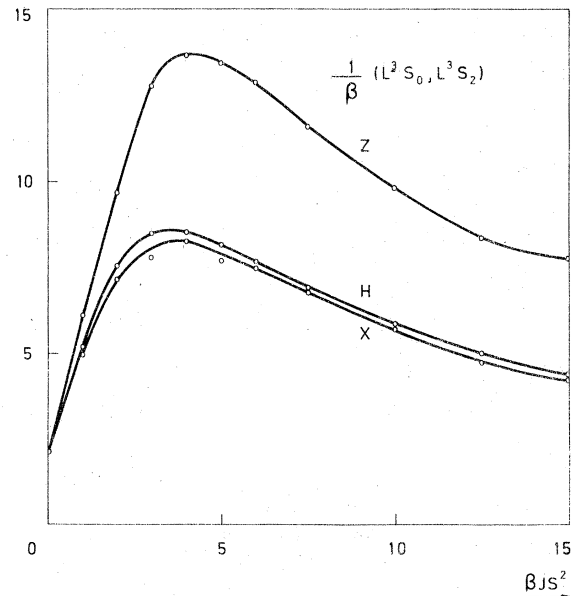
FIG. 7. Correlation function between the third time derivatives of next-nearest neighbors. See also Fig. 5.

FIG. 8. Inverse correlation length κ as a function of the inverse temperature βJS^2.
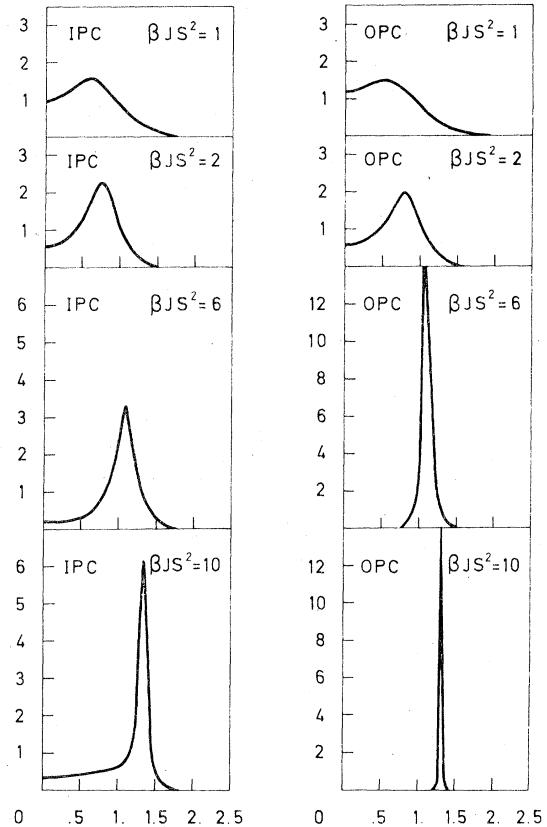

FIG. 9. Imaginary part of the normalized relaxation function for the in-plane (IPC) (left) and out-of-plane (OPC) (right) component for the wave vector $q = 0.35\pi$, and as a function of the inverse temperature βJS^2. The energy is measured in units of JS. It should be noted that for the two lowest temperatures the scale on the ordinate at the right-hand side differs from that of the left-hand side.

for the static correlation function. Because $\langle (S_n^a)^2 \rangle$ is directly given by the Monte Carlo calculation, only the parameter $\kappa_a(\beta)$ has to be fitted. $\kappa_a(\beta)$ is the inverse correlation length, and is a measure for the extension of the short-range order in the system. In Fig. 8, κ_x and κ_z are compared with the Heisenberg result κ_H. It is seen that κ_x and κ_H vanish at low temperatures, and thus the zero wave-vector susceptibility diverges. κ_z on the contrary remains finite, and thus S^z is no critical variable.

From Figs. 2–7 it is seen that the moments of the in-plane component deviate very little from the Heisenberg results. The moments of the out-of-plane component however differ considerably at the lower temperatures. From the essentially different behavior of the susceptibilities for the out-of-plane component, compared with the in-plane component, it can be expected that the two relaxation functions will also differ considerably. This is confirmed in Fig. 9. We have chosen a typical wave vector $(q = 0.35\pi)$ and plotted the imaginary part of both components of the normalized relaxation function. At low temperatures the line width of the z component is much smaller than the line width of the in-plane component. At $\beta JS^2 = 10$, the z line width is even so small, that we can consider the excitations of the z component as free particles. At low temperatures the frequency is the same for both components.[6,11] The difference in the line shape between the two components disappears gradually if we go to higher temperatures. Also

interesting to note is the renormalization of the frequency. At higher temperatures there is a shift to lower frequencies for both components. This was also found by Steiner et al.[4] although they found a smaller shift. At $\beta JS^2 = 1$, the inverse correlation length κ is more or less equal to the wave vector $q = 0.35\pi$ for both components. The simple spin-wave picture expects the spin waves to disappear around this temperature. This is confirmed by Fig. 9.

Finally we remark that we have not made a quantitative comparison with experiments for $CsNiF_3$, because we believe that extensive and accurate experimental data for small wave vectors should be available in order to get a feeling for the importance of the quantum effects in this spin one magnet. However, it is interesting to note that there is a good qualitative agreement between theory and experiment. The results, presented in

Figs. 1–9, were made for chains of 200 spins.

ACKNOWLEDGMENTS

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