ON THE THEORY
OF ONE-DIMENSIONAL SPIN ½ SYSTEMS

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Proefschrift

ter verkrijging van de graad van doctor in
de wiskunde en natuurwetenschappen aan de
Rijksuniversiteit te Leiden, op gezag van
de Rector Magnificus Dr. A.E. Cohen,
hoogleraar in de faculteit der letteren,
volgens besluit van het college van dekanen
te verdedigen op woensdag 16 juni 1976
te klokke 16.15 uur

door

Eduard Johan van Dongen

geboren te Den Haag in 1947

1976

Krips Repro - Meppel

Promotor: Dr. H.W. Capel

Aan mijn ouders.

CONTENTS

Chapters I and II have appeared before in Physica as
H.W. Capel, E.J. van Dongen and Th.J. Siskens, Physica 76 (1974) 445.
E.J. van Dongen, H.W. Capel and Th.J. Siskens, Physica 79A (1975) 617.
(Physica is published by The North-Holland Publishing Co., Amsterdam).

INTRODUCTION AND SUMMARY

One of the important problems in statistical mechanics is the calculation of thermodynamic properties of a many-body system starting from the microscopic interactions between the constituent particles. The basic quantity to be evaluated is the logarithm of the partition function (or the free energy) of the system per particle, from which other thermodynamic quantities can be obtained. In many cases, however, an exact calculation is impossible. Therefore it can be of interest to consider relatively simple model systems, for which exact results can be derived. This thesis deals with some aspects of one-dimensional quantum systems with spin $S = \frac{1}{2}$ characterized by the hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \left[2(J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) - (b_x S_i^x + b_y S_i^y + b_z S_i^z) \right], \quad (\vec{S}_{N+1} \equiv \vec{S}_1). \qquad (1)$$

Here J_x, J_y and J_z are the exchange coupling constants between the x, y and z components of two neighbouring spins, and b_x, b_y and b_z are the components of an applied magnetic field $\vec{b}$.

The investigation of one-dimensional quantum spin systems may be of interest both from an experimental and from a theoretical point of view. Recently many experimental data have been obtained for three-dimensional systems, with the property that they can be decomposed into a set of one-dimensional chains with a large exchange coupling between neighbouring atoms belonging to the same chain and a much weaker coupling between atoms belonging to different chains. For a review see the paper of de Jongh and Miedema 1); for recent experimental work see e.g. the theses by van Tol 2) and Klaaijsen 3). At low temperatures the coupling between the chains can give rise to long-range magnetic ordering and the system behaves essentially as a two- or three-dimensional system *). For temperatures well above the transition temperature, the system can be described essentially in terms of a one-dimensional system characterized by the hamiltonian (1).

Near the transition temperature the physical properties of the system will depend in most cases only on some global characteristics such as e.g. the dimensionality of the system, the spatial symmetry of the exchange tensor

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*) Under suitable conditions, however, certain features of a one-dimensional antiferromagnetic chain may be observed below the transition temperature (K.M. Diederix and T.O. Klaassen, private communication).

and the range of the interactions, in view of universality and scaling 4),5). Above the critical temperature, however, the physical properties can depend on the details of the interaction to a large extent.

Finally it should be mentioned that in a number of cases a relation has been derived between the ground state of the hamiltonian of a one-dimensional spin model and the largest eigenvalue of the transfer matrix of a two-dimensional vertex model. For a review, see Kasteleyn 6).

For some special cases of the hamiltonian (1) an exact treatment has been given. As examples the following models can be mentioned:

1. The one-dimensional Ising model 7) with a parallel field ($J_y = J_z = 0$; $b_y = b_z = 0$). For some details on the free energy and correlation functions, see Domb 8) and Thompson 9).

2. The XY model ($J_z = 0$) with a perpendicular field ($b_x = b_y = 0$), which includes the special case of the Ising model ($J_y = J_z = 0$) with a perpendicular field. The equilibrium properties have been derived by Lieb, Schultz and Mattis 10) and by Katsura 11), the non-equilibrium properties by Niemeijer 12).

3. The XXZ model ($J_x = J_y$) and the XYZ model. The exact solution for the ground state of the general XYZ model with three different exchange parameters J_x, J_y and J_z in the absence of a magnetic field ($\vec{b} = 0$) has been obtained by Baxter 13). The special case with axial symmetry, the XXZ model, has been solved earlier by Yang and Yang 14).

Since the XY model plays an important role in the calculations of this thesis, it is worthwhile to discuss some aspects of this model in more detail. In 1961 Lieb, Schultz and Mattis 10) solved the XY model for zero temperature. One of the underlying features is that the hamiltonian can be expressed in terms of paulion operators $a_j^\dagger = S_j^x + iS_j^y$ and $a_j = S_j^x - iS_j^y$, ($j = 1, \ldots, N$), which satisfy fermion anticommutation relations if they refer to the same lattice site j and boson commutation relations if they refer to different lattice sites. Lieb et al. performed the Jordan-Wigner transformation 15), which replaces the paulion operators $a_j^\dagger$ and a_j by operators $c_j^\dagger$ and c_j satisfying fermion anticommutation relations. They expressed the hamiltonian (1) with $J_z = 0$, $b_x = b_y = 0$ and the spin-cyclic (or a-cyclic) boundary condition $\vec{S}_{N+1} \equiv \vec{S}_1$ in terms of the c operators. The result is an expression which is bilinear and cyclic in the c operators apart from a term which can be considered to be a boundary term. Omitting this term one finds a hamiltonian which is cyclic in the c operators and which defines the so-called c-cyclic XY model. This hamiltonian can be diagonalized easily using a Fourier transformation and a Bogoliubov transformation.

Katsura [11)] derived an exact expression which is valid at all temperatures for the free energy per particle in the thermodynamic limit. Niemeijer [12)] evaluated the time-dependent correlation functions of the z components of two spins and the time-autocorrelation function of the z component of the magnetization.

Mazur and Siskens [16),17),18)] investigated the relation between the spin-cyclic and c-cyclic version of the XY model in detail, also for finite chains. Using a projection operator technique they were able to express the canonical averages with respect to the spin-cyclic XY hamiltonian in terms of the canonical averages with respect to the c-cyclic and the so-called c-anticyclic hamiltonian. (In the c-anticyclic hamiltonian the coupling constant between the c operators referring to sites N and 1 is equal to minus the coupling constant referring to two neighbouring sites j and j+1, in contrast with the c-cyclic case, where the coupling between sites N and 1 has the same sign.)

In chapter I of this thesis the time-dependent correlation functions have been investigated and a high-temperature expansion up to the order β^6 ($\beta \equiv (kT)^{-1}$) has been given for the element χ_{xx} of the susceptibility tensor of the spin-cyclic XY chain. Applying the projection operator technique mentioned above to the calculation of χ_{xx}, one has to evaluate averages of products of operators, which contain in particular a factor involving the c-cyclic as well as the c-anticyclic hamiltonian. This factor which does not arise in the calculation of the zz correlation functions prevents a rigorous calculation of the time-dependent xx correlation functions. In contrast with χ_{zz}, the high-temperature expansion of χ_{xx} shows a strong dependence on the anisotropy. It is also shown that the expression for χ_{xx} is different from its c-cyclic counterpart, even in the thermodynamic limit.

At the end of chapter I two remarks have been added. The first one deals with a simple proof of the thermodynamic Wick theorem [19),20)] for fermion operators, which has been used extensively in the calculation of the correlation functions. The second remark illustrates the difference between the spin-cyclic and c-cyclic version of the XY model for the special case of the Ising model [21)]. For the c-cyclic version of the Ising model exact results are given for the susceptibility χ_{xx} and the autocorrelation function per particle of the x component of the magnetization; the latter quantity turns out to be time-dependent.

Very recently, Amit Sur, Jasnow and Lowe [22)] studied the autocorrelation function of the x component of the magnetization in the high-temperature limit for $b_z = 0$. On the basis of finite chain calculations they conjectured that the autocorrelation function of the infinite isotropic XY chain has a Gaussian dependence on time. So far no analytical proof of this conjecture has been obtained.

Chapter II deals with the anisotropic spin ½ Heisenberg chain (J_x, J_y and J_z being different) with nearest-neighbour interactions, cf. eq. (1). Katsura and Inawashiro [23)] used a perturbation calculation in terms of J_z for the logarithm of the partition function per particle, starting from the isotropic XY hamiltonian. Using a quite different approach Baker, Rushbrooke and Gilbert [24)] derived high-temperature expansions for the logarithm of the partition function per particle and the susceptibility χ in zero field for the isotropic Heisenberg chain ($J_x = J_y = J_z$). Wood and Dalton [25)] and Jou and Chen [26)] have derived high-temperature expansions in the case of axial symmetry ($J_x = J_y$) which apply also to more general spins and lattices.

In chapter II the specific heat and the susceptibility χ_{zz} per particle in zero field are given up to β^9 and β^6 resp. In particular use is made of a first order perturbation calculation in J_z and the exact results of the anisotropic XY model. Note that within the context of the derivation of a high-temperature expansion all integrals occurring in expressions for correlation functions of the XY model become trivial. Furthermore use is made of the high-temperature expansion for χ_{xx} of the XY model and the high-temperature expansion for the susceptibility of the isotropic Heisenberg chain. Finally the numerical calculations for finite Heisenberg chains with axial symmetry should be mentioned. These calculations give quite accurate results in the thermodynamic limit, cf. Bonner and Fisher [27)] and also Blöte [28)] and de Neef and Hijmans [29)] for more recent results.

In chapter I and II high-temperature expansions have been given for physical quantities of the XY model and the more general XYZ model resp. Chapter III, on the other hand, deals with results for the Ising chain ($J_y = J_z = 0$) which are valid at all temperatures. Exact expressions are given for the (diagonal) elements of the susceptibility tensor in the presence of a parallel or perpendicular magnetic field b_x or b_z, apart from the parallel susceptibility χ_{xx} in a field b_z which is evaluated using a perturbation calculation (Also the elements of the staggered susceptibility tensor are given). As a result it is found that at sufficiently low temperatures all susceptibilities of an antiferromagnetic Ising chain ($J > 0$) show a minimum for $\vec{b} = 0$ and consequently a maximum at some finite value of the magnetic field. For high temperatures the susceptibilities have a maximum for $\vec{b} = 0$ (The staggered susceptibilities, on the other hand, have a maximum for $\vec{b} = 0$ at all temperatures).

Finally, the possibility of a relation between the susceptibilities of the one-dimensional Ising chain and the curious form of the phase boundary corresponding to the transition from antiferromagnetism to paramagnetism as observed by van Tol and Poulis 2),30) is discussed from a qualitative point of view.

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I. ON THE TRANSVERSE SUSCEPTIBILITY χ_{xx} OF THE ANISOTROPIC ONE-DIMENSIONAL *XY* MODEL IN THE PRESENCE OF A MAGNETIC FIELD IN THE *z* DIRECTION

1. *Introduction.* The one-dimensional anisotropic *XY* model was introduced by Lieb, Schultz and Mattis[1]) in 1961. Katsura[2]) evaluated an exact expression for the free energy, also in the presence of a nonzero magnetic field in the *z* direction. Niemeijer[3]) derived the time correlation functions of the *z* components of two spins. From refs. 2 and 3 one can obtain an expression for the longitudinal susceptibility *i.e.* the *zz* component of the susceptibility tensor.

In ref. 3 the spin correlation functions have been calculated for the so-called c-cyclic *XY* model, but in the thermodynamic limit these correlation functions can be shown to be equal to those for the so-called a-cyclic *XY* model, which is cyclic in the spins. A detailed investigation of the relation between the a-cyclic and the c-cyclic (or c-anticyclic) model has been given in refs. 4, 5 and 6. In ref. 5 it was shown in particular that the time-dependent *zz* correlation functions in the a-cyclic model can be expressed in terms of canonical averages referring to the c-cyclic or c-anticyclic hamiltonian.

The calculation of the transverse susceptibility (*i.e.*, the *xx* or *yy* components of the susceptibility tensor) is much more difficult, since, as will be shown later on in this paper, the canonical averages involve both the c-cyclic and the c-anticyclic hamiltonian. This difficulty does not show up in the calculation of the time-independent *xx* or *yy* correlation functions, *cf.* ref. 1 for $T = 0$ and refs. 7 and 8 for nonzero temperatures. Time-dependent correlation functions have also been considered by McCoy *et al.* for $T = 0$ in two asymptotic cases related to the time and the distance between the spins[9]).

In the present paper we give a high-temperature series expansion for the transverse susceptibility χ_{xx} in the thermodynamic limit using expansions for the xx spin correlation functions for imaginary times (in the absence of a magnetic field in the x direction).

In section 2 we review some properties of the a-cyclic XY model as given in refs. 4 and 5, which are relevant for the present calculation. In section 3 we express the xx spin correlation functions in terms of canonical averages involving the density operators of the c-cyclic and the c-anticyclic models. However, in the case of xx correlation functions, we must evaluate averages of complicated operators, which contain in particular a factor involving the c-cyclic as well as the c-anticyclic hamiltonian. This factor prevents a rigorous calculation of the time-dependent xx spin correlation functions. In section 4 this factor is investigated in detail and in particular those aspects which are relevant for the calculation of the high-temperature expansion for χ_{xx} up to a certain order. In section 5 we calculate the transverse susceptibility up to order β^6, ($\beta = 1/kT$). In the calculation use is made of the thermodynamic Wick theorem in a version due to Bloch and De Dominicis[10]).

In section 6 we give a few graphs and also a discussion on some aspects which can be of interest, such as the dependence on the inverse temperature β, the magnetic field B and the anisotropy parameter γ. In section 7, we give a high-temperature expansion for the susceptibility χ_{xx} of the c-cyclic XY model. The result turns out to be different from the transverse susceptibility in the a-cyclic model, even in the thermodynamic limit. This demonstrates in an explicit way the difficulties which can arise, if one uses the c-cyclic model for the calculation of physical quantities, even in the thermodynamic limit.

2. *Review of the a-cyclic XY model.* We consider a linear chain of N spins $\frac{1}{2}$ in an external homogeneous magnetic field B along the z axis. The spins have anisotropic nearest-neighbour interactions. The hamiltonian of the system (the so-called XY model) is given by

$$\mathscr{H} = \sum_{j=1}^{N} [(1 + \gamma)\, S_j^x S_{j+1}^x + (1 - \gamma)\, S_j^y S_{j+1}^y - B S_j^z], \tag{2.1}$$

where

$$S_{N+1}^x \equiv S_1^x \qquad \text{and} \qquad S_{N+1}^y \equiv S_1^y. \tag{2.2}$$

Performing the transformation to paulion operators

$$S_j^x = \tfrac{1}{2}(a_j^\dagger + a_j), \qquad S_j^y = (a_j^\dagger - a_j)/2\mathrm{i},$$

$$S_j^z = a_j^\dagger a_j - \tfrac{1}{2} \qquad (j = 1, \ldots, N) \tag{2.3}$$

and subsequently the Jordan–Wigner transformation

$$\begin{aligned} a_j^\dagger &= \exp\left(\mathrm{i}\pi\sum_{k=1}^{j-1} c_k^\dagger c_k\right) c_j^\dagger, \qquad (j = 2, \dots, N), \qquad a_1^\dagger = c_1^\dagger, \\ a_j &= \exp\left(-\mathrm{i}\pi\sum_{k=1}^{j-1} c_k^\dagger c_k\right) c_j, \qquad (j = 2, \dots, N), \qquad a_1 = c_1, \end{aligned} \tag{2.4}$$

the hamiltonian assumes the form

$$\begin{aligned} \mathscr{H} &= \tfrac{1}{2}NB - B\sum_{j=1}^{N} c_j^\dagger c_j + \tfrac{1}{2}\sum_{j=1}^{N} [(c_j^\dagger c_{j+1} + \gamma c_j^\dagger c_{j+1}^\dagger) + \text{h.c.}] \\ &\quad - \tfrac{1}{2}[(c_N^\dagger c_1 + \gamma c_N^\dagger c_1^\dagger) + \text{h.c.}]\left[\exp\left(\mathrm{i}\pi\sum_{j=1}^{N} c_j^\dagger c_j\right) + 1\right], \qquad (c_{N+1} \equiv c_1), \end{aligned} \tag{2.5}$$

where the c operators satisfy fermion anticommutation relations.

The model under consideration is cyclic in the spin operators and consequently in the a operators. It is therefore called the a-cyclic XY model.

It is, however, not cyclic in the c operators. By neglecting the last term in the right-hand side of (2.5) one obtains the so-called c-cyclic XY model, which is much easier to handle. For certain quantities it can be shown that in the thermodynamic limit the c-cyclic and the a-cyclic XY models give the same results, *cf.* refs. 4–6. (This can of course not be true for finite systems.) In the present paper it will be shown that this simplification is not always correct, even in the thermodynamic limit. For this purpose we shall present a detailed investigation of the transverse susceptibility, corresponding to an infinitesimal magnetic field in the x direction.

The a-cyclic hamiltonian (2.1) can be written

$$\mathscr{H} = \mathscr{H}_{-1} + \tfrac{1}{2}h(P + 1), \tag{2.6}$$

where the c-cyclic hamiltonian $\mathscr{H}_{-1}$ is given by

$$\mathscr{H}_{-1} = \tfrac{1}{2}NB - B\sum_{j=1}^{N} c_j^\dagger c_j + \tfrac{1}{2}\sum_{j=1}^{N} [(c_j^\dagger c_{j+1} + \gamma c_j^\dagger c_{j+1}^\dagger) + \text{h.c.}] \tag{2.7}$$

and where h and P are defined as

$$h = -[(c_N^\dagger c_1 + \gamma c_N^\dagger c_1^\dagger) + \text{h.c.}] \tag{2.8}$$

and

$$P = \exp\left(\mathrm{i}\pi\sum_{j=1}^{N} c_j^\dagger c_j\right). \tag{2.9}$$

We now define operators P_σ for $\sigma = \pm 1$ by

$$P_\sigma = \tfrac{1}{2}(1 + \sigma P), \tag{2.10}$$

where 1 is the unit operator. The operators P_σ are projection operators, *i.e.*

$$P_\sigma^2 = P_\sigma \qquad (\sigma = \pm 1), \tag{2.11}$$

which is obvious from the trivial relation

$$P^2 = 1. \tag{2.12}$$

In addition they have the following properties

$$P_\sigma P_{-\sigma} = 0 \qquad (\sigma = -1, 1), \tag{2.13}$$

$$[P_\sigma, \mathscr{H}_{-1}] = 0 \qquad (\sigma = -1, 1), \tag{2.14}$$

$$[P_\sigma, h] = 0 \qquad (\sigma = -1, 1). \tag{2.15}$$

Eqs. (2.14) and (2.15) are obvious, since P commutes with $\mathscr{H}_{-1}$ and h.

From the relation

$$\mathscr{H} = \mathscr{H}_{-1} + hP_1, \tag{2.16}$$

it follows immediately that

$$P_\sigma \mathscr{H} = P_\sigma \mathscr{H}_\sigma \qquad (\sigma = -1, +1), \tag{2.17}$$

where $\mathscr{H}_1$ is the hamiltonian of the so-called c-anticyclic model, defined by

$$\mathscr{H}_1 = \mathscr{H}_{-1} + h. \tag{2.18}$$

More generally, if f is an analytic function, then

$$P_\sigma f(\mathscr{H}) = P_\sigma f(\mathscr{H}_\sigma) \qquad (\sigma = -1, 1). \tag{2.19}$$

In order to evaluate physical quantities involving canonical averages for the a-cyclic XY model, one can introduce the projection operators P_σ by the trivial relation

$$\sum_\sigma P_\sigma = 1. \tag{2.20}$$

Using the projection and (anti)commutation properties of the operators P_σ, averages for the a-cyclic XY model can always be expressed in terms of averages with respect to the c-cyclic and the c-anticyclic hamiltonian.

Before we do this, we shall briefly review the c-cyclic and c-anticyclic XY model. These models can be conveniently described in terms of hermitean operators α_j and β_j ($j = 1, \ldots, N$), which are linear combinations of the c operators, *viz.*,

$$\alpha_j = \frac{1}{\sqrt{2}}(c_j + c_j^\dagger), \qquad \beta_j = \frac{-\mathrm{i}}{\sqrt{2}}(c_j - c_j^\dagger) \qquad (j = 1, \ldots, N) \tag{2.21}$$

and which have the anticommutation relations

$$\{\alpha_i, \alpha_j\} = \delta_{ij}, \qquad \{\beta_i, \beta_j\} = \delta_{ij},$$
$$\{\alpha_i, \beta_j\} = 0 \qquad (i, j = 1, \ldots, N). \tag{2.22}$$

The hamiltonians $\mathscr{H}_\sigma$ ($\sigma = -1, +1$) can now be expressed as

$$\mathscr{H}_\sigma = i \sum_{j,k=1}^{N} (S_\sigma)_{jk}\, \alpha_j \beta_k, \tag{2.23}$$

where the matrices S_σ (S_{-1} is cyclic and S_1 is anticyclic) are given by

$$(\mathsf{S}_\sigma)_{jk} = (\mathsf{S}_\sigma)_{k-j} \tag{2.24}$$

and

$$(\mathsf{S}_\sigma)_n = -B\delta_{n,0} + \tfrac{1}{2}(1 - \gamma)\,\delta_{n,1} - \tfrac{1}{2}\sigma(1 - \gamma)\,\delta_{n,1-N}$$
$$+ \tfrac{1}{2}(1 + \gamma)\,\delta_{n,-1} - \tfrac{1}{2}\sigma(1 + \gamma)\,\delta_{n,N-1}. \tag{2.25}$$

Here n runs from $1 - N$ to $N - 1$.

The dynamics of both models can be solved easily in terms of the α and β operators. We have the relations

$$\alpha_j(\tau, \sigma) = \sum_{k=1}^{N} [(\cosh \mathsf{M}_\sigma^{\frac{1}{2}}\tau)_{jk}\, \alpha_k - \mathrm{i}\,(\mathsf{S}_\sigma \mathsf{M}_\sigma^{-\frac{1}{2}} \sinh \mathsf{M}_\sigma^{\frac{1}{2}}\tau)_{jk}\, \beta_k],$$
$$(\sigma = -1, 1; j = 1, \ldots, N); \tag{2.26}$$

$$\beta_j(\tau, \sigma) = \sum_{k=1}^{N} [(\cosh \mathsf{M}_\sigma^{\frac{1}{2}}\tau)_{jk}\, \beta_k + \mathrm{i}\,(\tilde{\mathsf{S}}_\sigma \mathsf{M}_\sigma^{-\frac{1}{2}} \sinh \mathsf{M}_\sigma^{\frac{1}{2}}\tau)_{jk}\, \alpha_k],$$
$$(\sigma = -1, 1; j = 1, \ldots, N); \tag{2.27}$$

where $O(\tau, \sigma)$ for an arbitrary operator O is defined by

$$O(\tau, \sigma) \equiv \exp(\tau \mathscr{H}_\sigma)\, O \exp(-\tau \mathscr{H}_\sigma) \qquad (\sigma = -1, 1), \tag{2.28}$$

and where $\tilde{\mathsf{S}}_\sigma$ is the transpose matrix of S_σ, and M_σ is defined by

$$\mathsf{M}_\sigma \equiv \mathsf{S}_\sigma \tilde{\mathsf{S}}_\sigma = \tilde{\mathsf{S}}_\sigma \mathsf{S}_\sigma \qquad (\sigma = -1, 1). \tag{2.29}$$

The matrices M_σ are symmetric (M_{-1} is cyclic and M_{+1} is anticyclic). The relations (2.26) and (2.27) can be obtained from eqs. (24) and (25) in ref. 4 by substituting $t = -\mathrm{i}\tau$.

The reason for introducing the α and β operators lies in the simple expression (2.23) for the hamiltonian $\mathscr{H}_\sigma$. This expression is not only convenient for the solution (2.26)–(2.27) of the equations of motion, but, as we shall see later on, it enables us to apply Wick's theorem in a convenient way without performing the transformation to the representation in which $\mathscr{H}_\sigma$ is diagonal.

We finally express the components of the spin operators in terms of the α and β operators.

Using (2.3), (2.4) and (2.21) we have

$$S_1^x = \frac{\alpha_1}{\sqrt{2}}, \qquad S_j^x = \left(\prod_{k=1}^{j-1} \frac{2}{\mathrm{i}}\, \alpha_k \beta_k\right) \frac{\alpha_j}{\sqrt{2}} \qquad (j = 2, \ldots, N), \tag{2.30}$$

$$S_1^y = -\frac{\beta_1}{\sqrt{2}}, \qquad S_j^y = -\left(\prod_{k=1}^{j-1} \frac{2}{\mathrm{i}}\, \alpha_k \beta_k\right) \frac{\beta_j}{\sqrt{2}} \qquad (j = 2, \ldots, N), \tag{2.31}$$

$$S_j^z = \mathrm{i}\alpha_j \beta_j \qquad (j = 1, \ldots, N). \tag{2.32}$$

From the anticommutation relations (2.22) it follows that the operator P, defined by eq. (2.9), and reading

$$P = \prod_{j=1}^{N} [(2/\mathrm{i})\, \alpha_j \beta_j], \tag{2.33}$$

anticommutes with the α and β operators, *i.e.*,

$$\{P, \alpha_j\} = 0, \qquad \{P, \beta_j\} = 0 \qquad (j = 1, \ldots, N). \tag{2.34}$$

Consequently, P anticommutes with S_j^x and S_j^y and commutes with S_j^z, *viz.*,

$$\{P, S_j^x\} = 0, \qquad \{P, S_j^y\} = 0 \qquad (j = 1, \ldots, N), \tag{2.35}$$

$$[P, S_j^z] = 0 \qquad (j = 1, \ldots, N). \tag{2.36}$$

For the projection operators P_σ we therefore have the following properties

$$P_\sigma S_j^x = S_j^x P_{-\sigma} \qquad (\sigma = -1, 1; j = 1, \ldots, N), \tag{2.37}$$

$$P_\sigma S_j^y = S_j^y P_{-\sigma} \qquad (\sigma = -1, 1; j = 1, \ldots, N), \tag{2.38}$$

$$P_\sigma S_j^z = S_j^z P_\sigma \qquad (\sigma = -1, 1; j = 1, \ldots, N). \tag{2.39}$$

From eqs. (2.14), (2.15), (2.18), (2.19), (2.28) and (2.37), (2.38) and (2.39) we obtain the relations

$$\begin{aligned} P_\sigma S_j^x(\tau) &\equiv P_\sigma \exp(\tau \mathscr{H})\, S_j^x \exp(-\tau \mathscr{H}) = \exp(\tau \mathscr{H}_\sigma)\, P_\sigma S_j^x \exp(-\tau \mathscr{H}) \\ &= \exp(\tau \mathscr{H}_\sigma)\, S_j^x P_{-\sigma} \exp(-\tau \mathscr{H}) = \exp(\tau \mathscr{H}_\sigma)\, S_j^x \exp(-\tau \mathscr{H}_{-\sigma})\, P_{-\sigma} \\ &= S_j^x(\tau, \sigma) \exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})\, P_{-\sigma}, \\ &(\sigma = -1, 1; j = 1, \ldots, N); \end{aligned} \tag{2.40}$$

and similarly

$$\begin{aligned} P_\sigma S_j^y(\tau) &= S_j^y(\tau, \sigma) \exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})\, P_{-\sigma}, \\ &(\sigma = -1, 1; j = 1, \ldots, N); \end{aligned} \tag{2.41}$$

$$P_\sigma S_j^z(\tau) = S_j^z(\tau, \sigma)\, P_\sigma \qquad (\sigma = -1, 1;\ j = 1, \ldots, N). \tag{2.42}$$

Note that the anticommutation relations (2.35) lead to an additional factor $\exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})$ which contains the c-cyclic as well as the c-anticyclic hamiltonian. This factor prevents in general an exact calculation of time-dependent correlation functions involving the x and y components of the spins, in contrast with the zz correlation functions which have been calculated by Niemeijer[3]).

3. *Transverse susceptibility of the a-cyclic XY model.* In the presence of a magnetic field B_x in the x direction, the hamiltonian of the system is given by $\mathscr{H} - B_x M_x$, where $\mathscr{H}$ is the hamiltonian of the XY model given by eq. (2.1) and $M_x = \sum_{l=1}^{N} S_l^x$ is the x component of the magnetization operator.

The transverse susceptibility per particle for $B_x = 0$ in the thermodynamic limit is defined by the relation

$$\chi_{xx} \equiv \chi = \lim_{N\to\infty} \lim_{B_x\to 0} (\beta N)^{-1} \frac{\partial^2}{\partial B_x^2} \ln \operatorname{Tr}\, [\exp -\beta(\mathscr{H} - B_x M_x)]. \tag{3.1}$$

From eq. (3.1) one can derive the relation

$$\chi = \lim_{N\to\infty} \frac{1}{N} \langle \varrho \int_0^\beta \mathrm{d}\tau\, M_x(\tau)\, M_x \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{j,k=1}^{N} \langle \varrho \int_0^\beta \mathrm{d}\tau\, S_j^x(\tau)\, S_k^x \rangle . \tag{3.2}$$

In eq. (3.2) use has been made of the notation

$$\langle O \rangle \equiv \mathrm{Tr}\, O, \tag{3.3}$$

$$O(\tau) \equiv \exp(\tau \mathscr{H})\, O \exp(-\tau \mathscr{H}), \tag{3.4}$$

for an arbitrary operator O and

$$\varrho \equiv \exp(-\beta \mathscr{H}) \langle \exp(-\beta \mathscr{H}) \rangle^{-1}, \tag{3.5}$$

is the density operator corresponding to the hamiltonian (2.1).

In view of the translational invariance of the hamiltonian (2.1) and the boundary condition (2.2), the susceptibility can be written

$$\chi = \lim_{N\to\infty} \sum_{k=1}^{N} \langle \varrho \int_0^\beta \mathrm{d}\tau\, S_1^x(\tau)\, S_k^x \rangle . \tag{3.6}$$

The right-hand side of eq. (3.6) contains important contributions from the spins $k = N, N-1, N-2, \ldots$. These contributions can be related to those from $k = 2, 3, 4 \ldots$ by using the KMS property

$$\langle \varrho A(\tau)\, B \rangle = \langle \varrho B(\beta - \tau)\, A \rangle, \tag{3.7}$$

for arbitrary operators A and B. From (3.7), (2.1) and (2.2), we have

$$\langle \varrho S_1^x(\tau)\, S_{N-p}^x \rangle = \langle \varrho S_1^x(\beta - \tau)\, S_{p+2}^x \rangle \qquad (p = 0, 1, 2, \ldots) \tag{3.8}$$

and the susceptibility per particle is given by

$$\chi = \langle \varrho \int_0^\beta \mathrm{d}\tau\, S_1^x(\tau)\, S_1^x \rangle + 2 \sum_{p=1}^{\infty} \langle \varrho \int_0^\beta \mathrm{d}\tau\, S_1^x(\tau)\, S_{p+1}^x \rangle . \tag{3.9}$$

The right-hand side of eq. (3.9) contains canonical averages with respect to the a-cyclic hamiltonian. We do not know these averages *a priori*, but by using eq. (2.20) the averages can be expressed in terms of averages with respect to the c-cyclic and the c-anticyclic hamiltonian.

By using eq. (2.19) the spin correlation functions appearing in eq. (3.9) can be expressed as

$$\langle \varrho S_1^x(\tau)\, S_{q+1}^x \rangle = \Big(\sum_\sigma Z_\sigma \langle \varrho_\sigma P_\sigma \rangle\Big)^{-1}$$

$$\times \sum_\sigma Z_\sigma \langle \varrho_\sigma P_\sigma S_1^x(\tau)\, S_{p+1}^x \rangle \qquad (p = 0, 1, 2, \ldots), \qquad (3.10)$$

where

$$Z_\sigma \equiv \langle \exp(-\beta \mathscr{H}_\sigma) \rangle \qquad (\sigma = -1, 1) \qquad (3.11\mathrm{a})$$

and

$$\varrho_\sigma \equiv Z_\sigma^{-1} \exp(-\beta \mathscr{H}_\sigma) \qquad (\sigma = -1, 1), \qquad (3.11\mathrm{b})$$

are the partition function and the density operator of the c-cyclic and c-anticyclic models, respectively.

After applying eq. (2.40) with P_σ to $S_1^x(\tau)$ and with $P_{-\sigma}$ to S_{p+1}^x successively and using the explicit relation (2.10), eq. (3.10) can be written as

$$\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle = \frac{\sum_\sigma Z_\sigma \langle \varrho_\sigma S_1^x(\tau, \sigma) \exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})\, S_{p+1}^x (1 + \sigma P) \rangle}{\sum_\sigma Z_\sigma \langle \varrho_\sigma (1 + \sigma P) \rangle}$$

$$(p = 0, 1, 2, \ldots). \qquad (3.12)$$

By using eq. (2.30), the right-hand side of (3.12) can be expressed in terms of the operators α and β. The result is

$$\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle = \Big(\sum_\sigma Z_\sigma \langle \varrho_\sigma (1 + \sigma P) \rangle\Big)^{-1}$$

$$\times \Bigg[\tfrac{1}{2} \sum_\sigma Z_\sigma \langle \varrho_\sigma \alpha_1(\tau, \sigma) \exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})$$

$$\times \Big(\prod_{j=1}^{p} (2/\mathrm{i})\, \alpha_j \beta_j\Big)\, \alpha_{p+1} (1 + \sigma P) \rangle\Bigg] \qquad (p = 1, 2, \ldots).$$

$$(3.13)$$

(For $p = 0$, the factor $\prod \ldots$ should be replaced by the unit operator.)

One of the apparent complications in the right-hand side of eq. (3.13) is the occurrence of the factor $\exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})$ which contains the c-cyclic and the c-anticyclic hamiltonian. Such difficulties do not appear in the case of *zz* correlation functions $\langle \varrho S_1^z(\tau)\, S_{p+1}^z \rangle$, *cf.* the difference between eqs. (2.41) and (2.42).

In the special case of time-independent correlation functions with $\tau = 0$, the right-hand side of eq. (3.13) can be evaluated by using a modified version of

Wick's theorem due to Bloch and De Dominicis[10]), which does not involve time-ordered products of operators. This version can be formulated as follows.

Consider a one-particle hamiltonian

$$\mathscr{H} = \sum_k \lambda_k \eta_k^\dagger \eta_k, \tag{3.14}$$

where the η_k are fermion operators.

Let $A_1, A_2, \ldots, A_{2n}$ be arbitrary linear combinations of the creation and annihilation operators $\eta_k^\dagger$ and $\eta_{k'}$ and let $\varrho \equiv \exp(-\beta\mathscr{H}) \langle \exp(-\beta\mathscr{H}) \rangle^{-1}$ be the density operator, then

$$\langle \varrho A_1 A_2 \cdots A_{2n} \rangle = \sum_{j_1, j_2, \ldots, j_{n-1}} (-1)^{\nu(P)} \langle \varrho A_1 A_{j_1} \rangle \langle \varrho A_{i_2} A_{j_2} \rangle \cdots \langle \varrho A_{i_n} A_{j_n} \rangle, \tag{3.15}$$

where j_1 runs through the values $2, 3, \ldots, 2n$; i_2 is the smallest integer different from 1 and j_1; j_2 can have all values different from $1, j_1$ and i_2; i_3 is the smallest integer different from $1, j_1, i_2, j_2$; and so on. $\nu(P)$ is the sign of the permutation

$$\begin{pmatrix} 1 & j_1 & i_2 & j_2 & \cdots & i_n & j_n \\ 1 & 2 & & \cdots & & 2n-1 & 2n \end{pmatrix}.$$

The right-hand side of eq. (3.15) is by definition the pfaffian consisting of the triangular array of averages $\langle \varrho A_i A_j \rangle$ with $1 \leq i < j \leq 2n$. Hence

$$\begin{aligned} \langle \varrho A_1 A_2 \cdots A_{2n} \rangle &\equiv \mathrm{Pf}\,(A_1, A_2, \ldots, A_{2n}) \\ &= \mathrm{Pf} \begin{array}{llll} \langle \varrho A_1 A_2 \rangle & \langle \varrho A_1 A_3 \rangle \cdots \langle \varrho A_1 A_{2n-1} \rangle & & \langle \varrho A_1 A_{2n} \rangle \\ & \langle \varrho A_2 A_3 \rangle \cdots \langle \varrho A_2 A_{2n-1} \rangle & & \langle \varrho A_2 A_{2n} \rangle \\ & & \vdots & \\ & & \langle \varrho A_{2n-2} A_{2n-1} \rangle & \langle \varrho A_{2n-2} A_{2n} \rangle \\ & & & \langle \varrho A_{2n-1} A_{2n} \rangle . \end{array} \end{aligned} \tag{3.16}$$

The relation between the Wick theorem and pfaffians was first noted by Caianiello[11]). An elegant proof of the modified version eq. (3.15) was given by Gaudin[12]) and this formulation has also been used in previous treatments of the *XY* model, *cf.* Lieb, Schultz and Mattis[1]) and McCoy *et al.*[7-9]).

If $\tau = 0$, the right-hand side of eq. (3.13) can be evaluated in a straightforward way by noting that for each value of σ, *i.e.*, the c-cyclic case and c-anticyclic case respectively, the operators α and β can be expressed as linear combinations of the fermion creation and annihilation operators $\eta_{k\sigma}^{\dagger}, \eta_{k\sigma}$ that diagonalize the hamiltonian $\mathscr{H}_{\sigma}$, *cf.*, the appendix of ref. 5.

The result is then a pfaffian consisting of the averages $\langle \varrho_{\sigma} A_i A_j \rangle$, where the A_i and A_j correspond to operators α and β.

The averages $\langle \varrho_{\sigma} A_i A_j \rangle$ have been calculated previously by Mazur and Siskens[4]). The result is

$$\langle \varrho_{\sigma} \alpha_i \alpha_j \rangle = \tfrac{1}{2}\delta_{ij} \qquad (\sigma = -1, 1\; i, j = 1, \ldots, N), \tag{3.17}$$

$$\langle \varrho_{\sigma} \beta_i \beta_j \rangle = \tfrac{1}{2}\delta_{ij} \qquad (\sigma = -1, 1; i, j = 1, \ldots, N), \tag{3.18}$$

$$\langle \varrho_{\sigma} \alpha_i \beta_j \rangle = \tfrac{1}{2}\mathrm{i}\, (\mathsf{S}_{\sigma} \mathsf{M}_{\sigma}^{-\frac{1}{2}} \tanh \tfrac{1}{2}\beta \mathsf{M}_{\sigma}^{\frac{1}{2}})_{ij} \qquad (\sigma = -1, 1; i, j = 1, \ldots, N), \tag{3.19}$$

where the matrices S_{σ} and M_{σ} have been defined by eqs. (2.24), (2.25) and (2.29).

For $\tau = 0$ and finite values of β, *i.e.*, at nonzero temperature, it is obvious that the terms in eq. (3.13) involving the operator P do not give a contribution in the thermodynamic limit. In fact we then have an average of a product in which the number of different operators β_k is of order N. In view of Wick's theorem and eq. (3.19) this gives rise to a factor which has the order of magnitude $(\tanh \frac{1}{2}\beta \mathsf{M}_{\sigma}^{\frac{1}{2}})^N$. (We shall not go into the details of the time-independent correlations which have been calculated by Lieb, Schultz and Mattis[1]) for $T = 0$ and by McCoy *et al.* for nonzero temperatures[7,8]).)

We now consider eq. (3.13) in the case that $\tau \neq 0$. If we may neglect the factor $\exp(\tau \mathscr{H}_{\sigma}) \exp(-\tau \mathscr{H}_{-\sigma})$, there is no problem. Using the explicit solution (2.26) for $\alpha_1(\tau, \sigma)$ and Wick's theorem, the correlation function (3.13) can be expressed in terms of a finite pfaffian, since in the same way as above the operator P does not contribute in the thermodynamic limit. However, it will be shown in the present paper that it is by no means justified to neglect this factor.

Finally, it may be noted that McCoy *et al.*[9]) have also studied the behaviour of time correlation functions $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$ with $\tau = it$ for $T = 0$ in the two limiting cases $p \to \infty$, $t \ll p$, and $t \to \infty$, $p \ll t$, respectively. The effect of the factor $\exp(\tau \mathscr{H}_{\sigma}) \exp(-\tau \mathscr{H}_{-\sigma})$ could be avoided by considering four-spin correlation functions of the type $\langle \varrho S_1^x(\tau)\, S_j^x(\tau)\, S_k^x S_l^x \rangle$. Such correlation functions contain an even number of S^x operators with the same time dependence. Then from eqs. (2.14), (2.15), (2.18), (2.19) and (2.37) it can be seen that

$$P_{\sigma} S_i^x(\tau)\, S_j^x(\tau) = S_i^x(\tau, \sigma)\, S_j^x(\tau, \sigma)\, P_{\sigma} \tag{3.20}$$

and by using Wick's theorem the four-spin correlation functions can be expressed in terms of pfaffians. By choosing j and l in such a way that the distance between the spins j and i and between the spins l and k is sufficiently large, one can argue that in the thermodynamic limit the decoupling

$$\langle \varrho S_i^x(\tau)\, S_j^x(\tau)\, S_k^x S_l^x \rangle \sim \langle \varrho S_i^x(\tau)\, S_k^x \rangle \langle \varrho S_j^x(\tau)\, S_l^x \rangle \tag{3.21}$$

will lead to correct expressions for the spin correlation functions. The results obtained by McCoy *et al.* are based on asymptotic properties of Toeplitz determinants in the limit that the number of rows and columns tends to infinity.

In the following section we shall investigate the factor $\exp(\tau\mathscr{H}_\sigma)\exp(-\tau\mathscr{H}_{-\sigma})$.

4. *Time-dependent factor.* In this section we consider in detail the time-dependent factor $\exp(\tau\mathscr{H}_\sigma)\exp(-\tau\mathscr{H}_{-\sigma})$ occurring in eq. (3.13) for the spin correlation function. From (2.18) we have the relation

$$\mathscr{H}_{-\sigma} = \mathscr{H}_\sigma - \sigma h \qquad (\sigma = -1, 1) \tag{4.1}$$

and in order to handle the time-dependent factor we can apply a Dyson-series expansion to the operator $\mathscr{H}_{-\sigma}$. The result is

$$\begin{aligned}\exp(\tau\mathscr{H}_\sigma)\exp(-\tau\mathscr{H}_{-\sigma}) = 1 + \sum_{q=1}^{\infty} \sigma^q \int_0^\tau \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \\ \cdots \int_0^{\tau_{q-1}} \mathrm{d}\tau_q h(\tau_1, \sigma)\, h(\tau_2, \sigma) \cdots h(\tau_q, \sigma) \\ (\sigma = -1, 1).\end{aligned} \tag{4.2}$$

Since the operator h is only a local hamiltonian, with a finite operator norm $\|h\|$, it can be shown that the right-hand side of eq. (4.2) is always convergent. Some details of the proof will be given in appendix A.

We write

$$h \equiv \sum_{\varepsilon=1,N} \nu_\varepsilon \alpha_\varepsilon \beta_{N+1-\varepsilon}, \tag{4.3}$$

where

$$\nu_1 = -\mathrm{i}(1+\gamma), \qquad \nu_N = -\mathrm{i}(1-\gamma). \tag{4.4}$$

After inserting eq. (4.3) in eq. (4.2), the qth order of perturbation can be written as sum of the 2^q terms which are characterized by the values $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_q$ corresponding to the q factors h. Consider now the contribution of one of these 2^q terms to the numerator in the right-hand side of eq. (3.13). It can now easily be seen that the terms with the operator P do not give a contribution in the thermodynamic limit. In fact in view of eqs. (2.26) and (2.27) we can also apply Wick's theorem to the time-dependent operators $\alpha(\tau', \sigma)$, $\beta(\tau'', \sigma)$ and an arbitrary term of the resulting pfaffian contains at least $N - p - q$ different operators β, which in view of eq. (3.19), would lead to a contribution with the order of magnitude $(\tanh \frac{1}{2}\beta \mathrm{M}^{\frac{1}{2}})^{N-p-q}$.

After neglecting the terms with the operator P, the correlation function (3.13) can be written

$$\begin{aligned}\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle = \tfrac{1}{2} \sum_\sigma \Bigg[\frac{Z_\sigma}{Z_1 + Z_{-1}} \left(\frac{2}{\mathrm{i}}\right)^p \\ \times \Bigg(\mathrm{Pf}_\sigma (\alpha_1(\tau,\sigma), \alpha_1, \beta_1, \alpha_2, \beta_2, \ldots, \alpha_p, \beta_p, \alpha_{p+1}) \\ + \sum_{q=1}^{\infty} \sigma^q \int_0^\tau \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \cdots \int_0^{\tau_{q-1}} \mathrm{d}\tau_q \sum_{\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_q = 1, N} \nu_{\varepsilon_1} \nu_{\varepsilon_2} \cdots \nu_{\varepsilon_q} \\ \times \mathrm{Pf}_\sigma (\alpha_1(\tau,\sigma), \alpha_{\varepsilon_1}(\tau_1,\sigma), \beta_{N+1-\varepsilon_1}(\tau_1,\sigma), \\ \ldots, \alpha_{\varepsilon_q}(\tau_q,\sigma), \beta_{N+1-\varepsilon_q}(\tau_q,\sigma), \alpha_1, \beta_1, \ldots, \alpha_p, \beta_p, \alpha_{p+1}) \Bigg) \Bigg]. \end{aligned} \tag{4.5}$$

The pfaffians occurring in eq. (4.5) are defined by eq. (3.16), if the density operator ϱ is replaced by ϱ_σ, *i.e.*, the density operator corresponding to the c-cyclic and c-anticyclic models, for $\sigma = -1, +1$ respectively.

In the right-hand side of eq. (4.5) we can also omit the factor $\sum_\sigma Z_\sigma/(Z_1 + Z_{-1})$. This follows from the fact that each pfaffian Pf_σ occurring in eq. (4.5) multiplied with the corresponding factor σ^q is independent of σ, *i.e.*,

$$\sigma^q\, \mathrm{Pf}_\sigma(\cdots) \qquad \text{independent of } \sigma. \tag{4.6}$$

In order to prove eq. (4.6) we use Wick's theorem and we consider an arbitrary term of the pfaffian. This term involves a product of $q + p + 1$ averages $\langle \varrho_\sigma A(\tau,\sigma)\, A'(\tau',\sigma) \rangle$, where

$$A \equiv \alpha_i \quad \text{or} \quad \beta_i; \qquad A' \equiv \alpha_j \quad \text{or} \quad \beta_j. \tag{4.7}$$

For the subscripts i and j we have two possibilities:

$$\begin{aligned} &\text{a)} \quad i \text{ is an index of the order 1,} \quad \textit{i.e.} \quad i = \mathcal{O}(1), \quad \text{if} \quad i \ll N; \\ &\text{b)} \quad i \text{ is an index of the order } N, \quad \textit{i.e.} \quad i = \mathcal{O}(N), \quad \text{if} \quad N - i \ll N. \end{aligned} \tag{4.8}$$

Then by using eqs. (2.25), (2.26), (2.27) and (3.19), it can be seen that

$$\langle \varrho_\sigma A(\tau,\sigma)\, A'(\tau',\sigma) \rangle \qquad \text{independent of } \sigma, \text{ if } i \text{ and } j \text{ are both } \mathcal{O}(1) \text{ or } \mathcal{O}(N), \tag{4.9a}$$

$$\langle \varrho_\sigma A(\tau,\sigma)\, A'(\tau',\sigma) \rangle \qquad \text{proportional to } \sigma,$$

$$\text{if } i = \mathcal{O}(1), j = \mathcal{O}(N), \text{ or if } i = \mathcal{O}(N), j = \mathcal{O}(1). \tag{4.9b}$$

If we now consider an arbitrary term of a pfaffian corresponding to the qth order of perturbation, the number of averages (4.7) that are proportional to σ, *cf.* (4.9b), is equal to $q - 2Q$, where Q is the number of averages $\langle \varrho_\sigma A(\tau,\sigma) A'(\tau',\sigma)\rangle$ where i and j are both $\mathcal{O}(N)$. From this eq. (4.6) is obvious since $\sigma^q \sigma^{q-2Q} = 1$.

From eqs. (3.9) and (4.5) with the factor $\sum_\sigma Z_\sigma/(Z_1 + Z_{-1})$ omitted, we have a formal expression for the transverse susceptibility per particle. The actual evaluation of the right-hand side of (4.5), however, is extremely tedious. First of all, the number of pfaffians as well as the number of terms contained in each pfaffian increases rapidly with the order of perturbation. Secondly, the actual calculation of the factors $\langle \varrho_\sigma A(\tau, \sigma) A'(\tau', \sigma)\rangle$ with eqs. (2.26), (2.27) and (3.19) involves a rather cumbersome numerical integration. Finally we need all correlation functions for all values of $p \geq 0$, and the larger the p, the larger are the pfaffians.

In the present paper we shall restrict ourselves to a high-temperature expansion of the transverse susceptibility, up to a certain order ν, *i.e.*

$$\chi = \sum_{m=1} c_n \beta^m, \tag{4.10}$$

where $m \leq \nu$.

The spin correlation functions $\langle \varrho S_1^x(\tau) S_{p+1}^x\rangle$ can be expanded as power series in τ and β, *i.e.*,

$$\langle \varrho S_1^x(\tau) S_{p+1}^x\rangle = \sum_{\lambda,\mu} c_{\lambda,\mu}^{(p)} \tau^\mu \beta^\lambda \tag{4.11}$$

and in view of the condition $m \leq \nu$, we can restrict ourselves to values of λ and μ satisfying

$$\lambda + \mu \leq \nu - 1. \tag{4.12}$$

This has three advantages. First of all, we can restrict ourselves to a limited number of orders q of perturbation, in fact $q \leq \nu - 1$. Secondly, we can restrict ourselves to a finite number of neighbours, since, if q is limited and p is too large, we would have too many different operators β_k, each leading to an average $\langle \varrho_\sigma \alpha_l \beta_k\rangle$, which in view of (3.19) is at least of order $\beta = (kT)^{-1}$. Finally, in the calculation of the averages $\langle \varrho_\sigma A(\tau, \sigma) A'(\tau', \sigma)\rangle$, the matrices $(\cosh \mathsf{M}_\sigma^{\frac{1}{2}}\tau)$, $(\mathsf{S}_\sigma \mathsf{M}_\sigma^{-\frac{1}{2}} \sinh \mathsf{M}_\sigma^{\frac{1}{2}}\tau)$ and $(\mathsf{S}_\sigma \mathsf{M}_\sigma^{-\frac{1}{2}} \tanh \frac{1}{2}\beta \mathsf{M}_\sigma^{\frac{1}{2}})$, occurring in eqs. (2.26), (2.27) and (3.19), can be expanded as power series in τ and β, respectively, and all matrix elements up to a certain order ν can be calculated analytically.

Although the calculation of the correlation functions subjected to the condition (4.12) is straightforward using eq. (4.5), it will turn out to be convenient to use a slightly different method which avoids the multiple integrations over $\tau_1, \tau_2, \ldots, \tau_q$. We shall define a "Liouville" operator $\mathscr{L}_\sigma$ by its action on an arbitrary operator A, *viz.*

$$\mathscr{L}_\sigma A \equiv [\mathscr{H}_\sigma, A] + A\sigma h \qquad (\sigma = -1, 1), \tag{4.13}$$

i.e. $\mathscr{L}_\sigma$ consists of the commutator with $\mathscr{H}_\sigma$ and a multiplication on the right by the operator σh. From the definition of the operator

$$O(\tau, \sigma) \equiv \exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma}) \qquad (\sigma = -1, 1), \tag{4.14}$$

we have the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}\tau} O(\tau, \sigma) = [\mathscr{H}_\sigma, O(\tau, \sigma)] + O(\tau, \sigma)\sigma h \qquad (\sigma = -1, 1) \tag{4.15}$$

and in view of the definition (4.13), the formal solution of (4.15) is given by

$$O(\tau, \sigma) = \exp(\mathscr{L}_\sigma \tau) \qquad (\sigma = -1, 1). \tag{4.16}$$

For the spin correlation function (3.13) we have the expression

$$\langle \varrho S_1^x(\tau) S_{p+1}^x \rangle = \tfrac{1}{2} \langle \varrho_\sigma \alpha_1 (\tau, \sigma) \sum_{n=0}^{\infty} \frac{\mathscr{L}_\sigma^n \tau^n}{n!} \left(\prod_{j=1}^{p} \frac{2}{\mathrm{i}} \alpha_j \beta_j \right) \alpha_{p+1} \rangle. \tag{4.17}$$

Here use has been made of the fact that the terms involving the operator P and the factor $\sum_\sigma Z_\sigma/(Z_1 + Z_{-1})$ in eq. (4.5) can be omitted in the thermodynamic limit, *cf.* the discussion below eq. (4.4) and eq. (4.6). This implies in particular that the right-hand side of eq. (4.17) should be independent of σ. This conclusion can be verified explicitly by using eqs. (4.9a) and (4.9b) and the fact that an arbitrary term of $\mathscr{L}_\sigma^n$ which contains m operators α and β with an index $\mathcal{O}(N)$ is proportional to σ^m. This statement can be proved easily by induction.

The various powers of $\mathscr{L}_\sigma$ can be calculated directly using the commutation relations (2.22)

$$[\mathscr{H}_\sigma, \alpha_j] = -\mathrm{i} \sum_{k=1}^{N} (\mathrm{S}_\sigma)_{jk} \beta_k, \tag{4.18}$$

$$[\mathscr{H}_\sigma, \beta_j] = \mathrm{i} \sum_{k=1}^{N} (\mathrm{S}_\sigma)_{kj} \alpha_k \qquad (\sigma = -1, 1; j = 1, \ldots, N). \tag{4.19}$$

As a result, we have

$$\mathscr{L}_\sigma = \sigma h = -2\mathrm{i}\sigma (S_{-1} \alpha_1 \beta_N + S_1 \alpha_N \beta_1), \tag{4.20}$$

$$\begin{aligned} \mathscr{L}_\sigma^2 &= [\mathscr{H}_\sigma, \sigma h] + \sigma^2 h^2 \\ &= (S_{-1}^2 + S_1^2) - 2\sigma B (S_{-1} - S_1)(\alpha_1 \alpha_N - \beta_1 \beta_N) \\ &\quad + 2\sigma S_{-1} S_1 (\alpha_1 \alpha_{N-1} + \beta_1 \beta_{N-1} - \alpha_2 \alpha_N - \beta_2 \beta_N) \\ &\quad - 8 S_{-1} S_1 \alpha_1 \beta_N \alpha_N \beta_1, \end{aligned} \tag{4.21}$$

$$\mathscr{L}_\sigma^3 = [\mathscr{H}_\sigma, \mathscr{L}_\sigma^2] + \mathscr{L}_\sigma^2 \sigma h \qquad (\sigma = -1, 1). \tag{4.22}$$

Here S_{-1} and S_1 are shorthand notations for the matrix elements

$$(\mathrm{S}_\sigma)_{-1} \equiv S_{-1} = \tfrac{1}{2}(1+\gamma), \qquad (\mathrm{S}_\sigma)_1 \equiv S_1 = \tfrac{1}{2}(1-\gamma). \tag{4.23}$$

The explicit formula for $\mathscr{L}_\sigma^3$ is rather complicated and is given in appendix B.

We now consider the general structure of $\mathscr{L}_\sigma^n$. By using the anticommutation relations (2.22) each operator α_k or β_l which occurs twice can be eliminated to give a factor $\pm\frac{1}{2}$, the sign depending on the number of interchanges that are needed to bring the two operators next to each other. Then $\mathscr{L}_\sigma^n$ can be written

$$\mathscr{L}_\sigma^n = \sum_{k,l} \sum_{i_1<i_2<\cdots<i_k} \sum_{j_1<j_2<\cdots<j_l} C^{(n)}_{i_1 i_2 \cdots i_k; j_1 \cdots j_l} \alpha_{i_1}\alpha_{i_2}\cdots\alpha_{i_k}\beta_{j_1}\cdots\beta_{j_l}. \tag{4.24}$$

If n increases, the number of operators $k+l$ involved in a term on the right-hand side can increase. This is due to the multiplication on the right by the operator σh; in each step two additional operators $\alpha_1\beta_N$ or $\alpha_N\beta_1$ will be added and if these operators do not occur in the original term, the number of operators will increase by 2. On the other hand, the number of operators α and β cannot increase, if we take the commutator $[\mathscr{H}_\sigma, \ldots]$. Hence, for increasing values of n, the powers $\mathscr{L}_\sigma^n$ can contain many operators α and β, which can be considered as many-body interactions within the context of the c-cyclic and the c-anticyclic XY models. This feature explains the complicated structure of the time-dependent correlation functions $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$.

The operators $\mathscr{L}_\sigma^n$ have the following two general properties:

a) if n is even, then $k = l$ is even, (4.25a)

if n is odd, then $k = l$ is odd; (4.25b)

b) consider a nonvanishing term in (4.24) with indices $i_1, i_2, \ldots, i_k$; $j_1, \ldots, j_l$.

From these indices $\frac{1}{2}(k+l)$ indices are of order $\mathcal{O}(1)$
the other $\frac{1}{2}(k+l)$ indices are of order $\mathcal{O}(N)$. (4.26)

The proof of eqs. (4.25) is trivial by induction. The proof of eq. (4.26) is somewhat more involved and will be given in appendix C.

We finally consider the contribution of an arbitrary term on the right-hand side of (4.24) to the spin correlation function (4.17). The contribution is proportional to

$$\tau^n \langle \varrho_\sigma \alpha_1(\tau,\sigma)\, \alpha_{i_1}\cdots\alpha_{i_k}\beta_{j_1}\cdots\beta_{j_l}\alpha_1\beta_1\alpha_2\beta_2\cdots\alpha_p\beta_p\alpha_{p+1} \rangle. \tag{4.27}$$

Using eq. (2.26) we can expand $\alpha_1(\tau,\sigma)$ as a power series in τ. Consider now the contribution due to an operator γ_l occurring in the rth-order term of this expansion. (Obviously $\gamma_l = \alpha_l$, if r is even and $\gamma_l = \beta_l$, if r is odd.) Then the contribution to the spin correlation function is proportional to

$$\tau^{n+r}\langle \varrho_\sigma \gamma_l \alpha_{i_1} \cdots \alpha_{i_k} \beta_{j_1} \cdots \beta_{j_l} \alpha_1 \beta_1 \alpha_2 \beta_2 \cdots \alpha_p \beta_p \alpha_{p+1} \rangle. \tag{4.28}$$

In order to evaluate the average in eq. (4.28), we eliminate all operators α and β which occur twice. Then we are left with an average of a product of operators α and β, each occurring once. The average can be different from 0, if the number s of different operators β is equal to the number of different operators α. Then the result can be expressed in terms of a $2s$-dimensional pfaffian, each term of which contains s contractions $\langle \varrho_\sigma \alpha_i \beta_j \rangle$. The pfaffian will have the order of magnitude $\beta^s = (kT)^{-s}$, provided that it contains at least one term so that in all the contractions $\langle \varrho_\sigma \alpha_i \beta_j \rangle$, $j - i = 0, \pm 1, \pm(N-1)$. If this is not the case the pfaffian will have at least the order of magnitude β^{s+2}. Thus one can evaluate in a systematic way all coefficients $c^{(p)}_{\lambda,\mu}$ in eq. (4.11) satisfying $\lambda + \mu \leq \nu - 1$, for a certain value of ν. (It may be noted that the $2s$-dimensional pfaffian obtained after removing the operators which occur twice, can also be written in terms of an $s \times s$ determinant, *cf.* Lieb, Schultz and Mattis. [In our calculation this will not be an important simplification, since in general in a sufficiently large pfaffian only a few terms will have an order in β that is low enough to satisfy eq. (4.12).])

In the following section we shall calculate the transverse susceptibility up to order β^6 ($\nu = 6$). We then can restrict ourselves to the terms $\tau^\mu \beta^\lambda$ in the spin correlation functions satisfying $\lambda + \mu \leq 5$.

5. *Correlation functions.* In this section we investigate the spin correlation functions (4.11) and we shall restrict ourselves to the terms $\tau^\mu \beta^\lambda$ with $\lambda + \mu \leq 5$. Instead of writing down complicated expressions for various powers of $\mathscr{L}^n_\sigma$, we shall select the terms that are relevant from our point of view, *i.e.* a term in the right-hand side of eq. (4.24) is called a "relevant term", if it can give a nonvanishing contribution $c^{(p)}_{\lambda\mu}\tau^\mu\beta^\lambda$ with $\lambda + \mu \leq 5$ to some spin correlation function $\langle \varrho S^x_1(\tau)\, S^x_{p+1} \rangle$. Obviously, in eq. (4.17), the terms $\mathscr{L}^n_\sigma$ with $n > 5$ are irrelevant.

We now consider $\mathscr{L}^5_\sigma$. In the average (4.27), we must take the 0-order term in the expansion of $\alpha_1(\tau, \sigma)$ in powers of τ, *i.e.* $\alpha_1(\tau, \sigma) = \alpha_1$. Then after eliminating the two operators α_1 occurring in eq. (4.27), all operators α and β should occur twice, otherwise we would have at least one additional factor of order $\beta = (kT)^{-1}$. This is not possible, however. [From (4.25) it follows that each term of $\mathscr{L}^5_\sigma$ contains an odd number of operators α and an odd number of operators β; from (4.26) it follows that at least one of the indices $i_1 \cdots i_k, j_1 \cdots j_l$ occurring in (4.27) must be of order $\mathcal{O}(N)$ and if $\alpha_1(\tau, \sigma) = \alpha_1$ each operator with an index $\mathcal{O}(N)$ occurs only once.] Hence, $\mathscr{L}^5_\sigma$ is "irrelevant".

We now turn to $\mathscr{L}^4_\sigma$. $\mathscr{L}^4_\sigma$ itself is of order τ^4, so that we only can have an additional factor τ, arising from the first-order term in τ in the expansion of $\alpha_1(\tau, \sigma)$, or an additional factor β, arising from one average $\langle \varrho_\sigma \alpha_i \beta_j \rangle$, where $j - i = 0, \pm 1, \pm(N-1)$.

First of all $\mathscr{L}^4_\sigma$ has a constant term which does not contain operators α and β. This term can give a contribution $\approx \tau^4$ to the autocorrelation function (4.27) with $p = 0$ and a contribution $\approx \tau^4 \beta$ to the nearest-neighbour correlation with $p = 1$. Obviously, the constant term can give no contributions $\approx \tau^5$, since the first-order term in the expansion of $\alpha_1(\tau, \sigma)$ involves operators $\beta_1, \beta_2, \beta_N$ and we are left with at least one average $\langle \varrho_\sigma \alpha_i \beta_j \rangle$ which would lead to an additional factor β. We now consider the terms which contain two operators $\alpha_i \alpha_j$. Obviously, from (4.26), j must be an index of order $\mathcal{O}(N)$. The first-order contribution of $\alpha_1(\tau, \sigma)$ involves operators β, so that we are left with an operator α_j, where $j = \mathcal{O}(N)$, which occurs only once in (4.27) and which would lead to at least one additional factor $\beta = (kT)^{-1}$. So we can restrict ourselves to terms with $\alpha_1(\tau, \sigma) = \alpha_1$, which lead to one average $\langle \varrho_\sigma \alpha_j \beta_k \rangle$ which is proportional to β. The only relevant term is $\alpha_2 \alpha_N$, giving a contribution $\approx \tau^4 \beta$ to the nearest-neighbour correlation with $p = 1$.

All terms $\beta_i \beta_j$ are irrelevant. If we consider the first-order contribution in τ of $\alpha_1(\tau, \sigma)$, we are left with the operator α_1 in (4.27) which would lead to an additional factor β. If we take the 0-order contribution, *i.e.* $\alpha_1(\tau, \sigma) = \alpha_1$, the two operators α_1 occurring in (4.27) can be eliminated. The operator β_j has an index $j = \mathcal{O}(N)$ and a nonvanishing contribution can only occur in an average $\langle \varrho_\sigma \beta_j \alpha_{p+1} \rangle$, where $p \geq 1$ and this average is at least of order $\mathcal{O}(\beta^3)$.

Finally we can consider operators $\alpha_i \alpha_j \beta_k \beta_l$ which contain two indices of order $\mathcal{O}(N)$. We can restrict ourselves to the terms with $\alpha_1(\tau, \sigma) = \alpha_1$ leading to an average $\langle \varrho_\sigma \alpha_j \beta_l \rangle$, where the indices j and l are both of order $\mathcal{O}(N)$. This gives an additional factor β. In addition all remaining operators in eq. (4.27) should occur twice. The only relevant terms are those for which $i = 2$, $k = 1$, *i.e.* the terms $\alpha_2 \alpha_j \beta_1 \beta_l$, where j and l are of order $\mathcal{O}(N)$; these terms can give a nonvanishing contribution $\approx \tau^4 \beta$ to the nearest-neighbour correlation with $p = 1$. In addition the difference $l - j$ should have one of the values $1, 0, -1$. If we now look at the complete expression for $\mathscr{L}^3_\sigma$, given in appendix B, we see that the only terms of this type that can arise after taking the commutator $[\mathscr{H}_\sigma, \ldots]$ or the multiplication at the right by σh are the terms $\alpha_2 \alpha_N \beta_1 \beta_N$ and $\alpha_2 \alpha_N \beta_1 \beta_{N-1}$.

Finally $\mathscr{L}^4_\sigma$ contains a few terms involving 4 operators α or 4 operators β; these terms can never give a contribution. As a conclusion all the terms of $\mathscr{L}^5_\sigma$ are irrelevant; the relevant terms in the expansion (4.24) of $\mathscr{L}^4_\sigma$ are given by

$$\text{constant term}, \qquad \alpha_2 \alpha_N, \qquad \alpha_2 \alpha_N \beta_1 \beta_N, \qquad \alpha_2 \alpha_N \beta_1 \beta_{N-1}. \tag{5.1}$$

A similar analysis can be given for the terms of $\mathscr{L}^3_\sigma$. Since we have given the complete expression in appendix B, we shall omit the details. The relevant terms of $\mathscr{L}^3_\sigma$ are

$$\alpha_1 \beta_N, \quad \alpha_N \beta_1, \quad \alpha_2 \beta_N, \quad \alpha_N \beta_2, \quad \alpha_N \beta_3, \quad \alpha_1 \alpha_2 \alpha_N \beta_N, \quad \beta_1 \beta_2 \beta_N \alpha_N. \tag{5.2}$$

Finally it can be shown that all the terms of $\mathscr{L}_\sigma^2$ and $\mathscr{L}_\sigma$, as given in eqs. (4.20) and (4.21) are relevant terms.

Using the relevant part of the operator $\exp(\mathscr{L}_\sigma \tau)$ the calculation of the spin correlation function is straightforward. Since the right-hand side of eq. (4.17) has been shown to be independent of σ, we shall from now on restrict ourselves to the value $\sigma = -1$. Using eqs. (5.1) and (5.2), the relevant part of $\exp \mathscr{L}_{-1}\tau$ is given by

$$\begin{aligned}\exp \mathscr{L}_{-1}\tau = 1 &+ 2\mathrm{i}\tau\,(S_{-1}\alpha_1\beta_N + S_1\alpha_N\beta_1) \\ &+ \tfrac{1}{2}\tau^2\,(c_0^{(2)} + c_1^{(2)}\alpha_1\alpha_N + c_2^{(2)}\beta_1\beta_N + c_3^{(2)}\alpha_1\alpha_{N-1} + c_4^{(2)}\beta_1\beta_{N-1} \\ &+ c_5^{(2)}\alpha_2\alpha_N + c_6^{(2)}\beta_2\beta_N + c_7^{(2)}\alpha_1\alpha_N\beta_1\beta_N) \\ &+ \tfrac{1}{6}\tau^3\,2\mathrm{i}\,(c_1^{(3)}\alpha_1\beta_N + c_2^{(3)}\alpha_N\beta_1 + c_3^{(3)}\alpha_2\beta_N + c_4^{(3)}\alpha_N\beta_2 \\ &+ c_5^{(3)}\alpha_N\beta_3 + c_6^{(3)}\alpha_1\alpha_2\alpha_N\beta_N + c_7^{(3)}\alpha_N\beta_1\beta_2\beta_N) \\ &+ \tfrac{1}{24}\tau^4\,(c_0^{(4)} + c_1^{(4)}\alpha_2\alpha_N + c_2^{(4)}\alpha_2\alpha_N\beta_1\beta_N + c_3^{(4)}\alpha_2\alpha_N\beta_1\beta_{N-1}).\end{aligned} \tag{5.3}$$

The coefficients $c^{(2)}$ and $c^{(3)}$ have been given in eq. (4.21) and appendix B. After substituting $\sigma = -1$, we have

$$\begin{aligned}&c_0^{(2)} = (S_{-1}^2 + S_1^2), \qquad c_1^{(2)} = -c_2^{(2)} = 2B\,(S_{-1} - S_1), \\ &c_3^{(2)} = c_4^{(2)} = -c_5^{(2)} = -c_6^{(2)} = -2S_{-1}S_1, \qquad c_7^{(2)} = -8S_{-1}S_1;\end{aligned} \tag{5.4}$$

$$\begin{aligned}&c_1^{(3)} = S_{-1}^3 + 5S_{-1}S_1^2 + 2B^2\,(S_{-1} - S_1), \\ &c_2^{(3)} = 5S_{-1}^2S_1 + S_1^3 - 2B^2\,(S_{-1} - S_1), \\ &c_3^{(3)} = -BS_{-1}\,(S_{-1} - S_1), \qquad c_4^{(3)} = BS_1\,(S_{-1} - S_1), \\ &c_5^{(3)} = S_{-1}S_1^2, \qquad c_6^{(3)} = 6S_{-1}^2S_1, \qquad c_7^{(3)} = 6S_{-1}S_1^2.\end{aligned} \tag{5.5}$$

The coefficients $c^{(4)}$ can be calculated by using the result for $\mathscr{L}_\sigma^3$ with $\sigma = -1$ in appendix B. $c_0^{(4)}$ is due to the multiplication of the terms with $\alpha_1\beta_N$, $\alpha_N\beta_1$ by σh. $c_1^{(4)}$ has a contribution from the term $\alpha_1\alpha_2\alpha_N\beta_N$ after multiplication by σh and also contributions from $\alpha_N\beta_1$, $\alpha_2\beta_N$, $\alpha_N\beta_2$, $\alpha_N\beta_3$ and $\alpha_2\beta_{N-1}$ after taking the commutator $[\mathscr{H}_\sigma, \ldots]$. $c_2^{(4)}$ can arise from the terms $\alpha_1\alpha_2\alpha_N\beta_N$ and $\alpha_N\beta_1\beta_2\beta_N$ by taking the commutator $[\mathscr{H}_\sigma, \ldots]$ and also from $\alpha_2\beta_N$ after multiplication by σh. Finally $c_3^{(4)}$ can be obtained from $\alpha_2\beta_{N-1}$ after multiplication by σh. The results are

$$\begin{aligned}&c_0^{(4)} = [S_{-1}^4 + 10S_{-1}^2S_1^2 + S_1^4 + 2B^2\,(S_{-1}^2 - 2S_{-1}S_1 + S_1^2)], \\ &c_1^{(4)} = [20S_{-1}^3S_1 + 4S_{-1}S_1^3 + 2B^2\,(-3S_{-1}^2 + 2S_{-1}S_1 + S_1^2)], \\ &c_2^{(4)} = -8B\,(S_{-1}^2S_1 - S_{-1}S_1^2), \qquad c_3^{(4)} = 8S_{-1}^2S_1^2.\end{aligned} \tag{5.6}$$

The spin correlation functions can be calculated by inserting (5.3)–(5.6) into eq. (4.17). We then use the expansion, *cf.* (2.26).

$$
\begin{aligned}
\alpha_1(\tau, -1) = \alpha_1 &- \mathrm{i}\tau\,(-B\beta_1 + S_1\beta_2 + S_{-1}\beta_N) \\
&+ \tfrac{1}{2}\tau^2\,[M_2(\alpha_3 + \alpha_{N-1}) + M_1(\alpha_2 + \alpha_N) + M_0\alpha_1] \\
&- \tfrac{1}{6}\mathrm{i}\tau^3\,[(\mathrm{SM})_3\,\beta_4 + (\mathrm{SM})_2\,\beta_3 + (\mathrm{SM})_1\,\beta_2 + (\mathrm{SM})_0\,\beta_1 \\
&+ (\mathrm{SM})_{-1}\,\beta_N + (\mathrm{SM})_{-2}\,\beta_{N-1} + (\mathrm{SM})_{-3}\,\beta_{N-2}] \\
&+ \tfrac{1}{24}\tau^4\,[(\mathrm{M}^2)_0\,\alpha_1 + (\mathrm{M}^2)_1\,\alpha_2 + \text{irrelevant terms}] \\
&+ \text{higher orders in } \tau.
\end{aligned}
\tag{5.7}
$$

Here M_q, $(\mathrm{SM})_q$ and $(\mathrm{M}^2)_q$, $|q| \leq 3$ are shorthand notations for matrix elements which are independent of σ, *i.e.*

$$
\begin{aligned}
&M_q \equiv (\mathrm{M}_\sigma)_{k\,k+q}, \qquad (\mathrm{SM})_q \equiv (\mathrm{S}_\sigma\mathrm{M}_\sigma)_{k\,k+q}, \\
&(\mathrm{M}^2)_q \equiv (\mathrm{M}_\sigma^2)_{k\,k+q}.
\end{aligned}
\tag{5.8}
$$

After inserting eqs. (5.3)–(5.7) into (4.17) we obtain a large number of terms, each containing an average of a product of operators α and β. Using Wick's theorem, the averages can be expressed in terms of pfaffians with elements $\langle\varrho_\sigma\alpha_i\beta_j\rangle$. To each element we apply the expansion

$$
\begin{aligned}
\langle\varrho_\sigma\alpha_k\beta_l\rangle &= \tfrac{1}{2}\mathrm{i}\,(\mathrm{S}_\sigma\mathrm{M}_\sigma^{-\frac{1}{2}}\tanh\tfrac{1}{2}\beta\mathrm{M}_\sigma^{\frac{1}{2}})_{l-k} \\
&= \frac{\mathrm{i}}{4}\,\beta\,(\mathrm{S}_\sigma)_{l-k} - \frac{\mathrm{i}\beta^3}{48}\,(\mathrm{S}_\sigma\mathrm{M}_\sigma)_{l-k} + \frac{\mathrm{i}\beta^5}{480}\,(\mathrm{S}_\sigma\mathrm{M}_\sigma^2)_{l-k},
\end{aligned}
\tag{5.9}
$$

for $\sigma = -1$.

For each value of p, (*i.e.* for each spin correlation function), we can combine the contributions that are proportional to $\tau^\mu\beta^\lambda$. We restrict ourselves to the values λ and μ satisfying $\lambda + \mu \leq 5$. This restriction reduces the number of neighbours we have to consider. In fact, in this approximation, we have

$$
\langle\varrho S_1^x(\tau)\,S_{p+1}^x\rangle = 0, \qquad \text{for} \qquad p \geq 6. \tag{5.10}
$$

[In this equation it has been assumed that $p \leq N - 5$, *cf.* eq. (3.8).] Furthermore, the restriction $\lambda + \mu \leq 5$ reduces to a large extent the size of the pfaffians we have to consider. The largest pfaffians have 4 or 5 rows, but they contain only one term which satisfies the restriction. Then we are left with pfaffians corresponding to 3 or less different operators α and different operators β; such pfaffians have at most 6 nonvanishing terms. The calculation of the spin correlation function is now straightforward, but very tedious. Some useful matrix elements are given in appendix D. The result can be expressed as

$$\langle \varrho S^x(\tau)\, S^x_{p+1} \rangle = A_p + B_p, \tag{5.11}$$

where A_p is the contribution from the term 1 on the right-hand side of (5.3) and B_p is the contribution from the remaining terms. The A_p are the correlation functions we would have obtained, if we had neglected the factor $e^{\tau\mathscr{H}_\sigma}\, e^{-\tau\mathscr{H}_{-\sigma}}$ in eq. (3.13). The explicit expressions for the coefficients A_p are given in appendix E. The coefficients B_p are given in appendix F. With these results the evaluation of the spin correlation functions with $p \leq 5$ is simple, and the result is

$$\langle \varrho S^x_1(\tau)\, S^x_6 \rangle = -\frac{\beta^5}{128} S^5_{-1}, \tag{5.12}$$

$$\langle \varrho S^x_1(\tau)\, S^x_5 \rangle = \frac{\beta^4}{64} S^4_{-1}, \tag{5.13}$$

$$\langle \varrho S^x_1(\tau)\, S^x_4 \rangle = -\frac{\beta^3}{32} S^3_{-1} + \frac{\beta^5}{384} (3S^5_{-1} + 5S^3_{-1}S^2_1 + 4B^2S^3_{-1}), \tag{5.14}$$

$$\langle \varrho S^x_1(\tau)\, S^x_3 \rangle = \frac{\beta^2}{16} S^2_{-1} - \frac{\beta^4}{192} (2S^4_{-1} + 4S^2_{-1}S^2_1 + 3B^2S^2_{-1}), \tag{5.15}$$

$$\begin{aligned}\langle \varrho S^x_1(\tau)\, S^x_2 \rangle = {} & -\frac{\beta}{8} S_{-1} + \frac{\beta^3}{96} [S^3_{-1} + 2S_{-1}S^2_1 + B^2(2S_{-1} + S_1)] \\ & + \frac{(\beta^2\tau - \beta\tau^2)}{16} (S_{-1}S^2_1 - B^2S_1) \\ & - \frac{\beta^5}{960} [S^5_{-1} + 6S^3_{-1}S^2_1 + 3S_{-1}S^4_1 + B^4(3S_{-1} + 2S_1) \\ & + B^2(6S^3_{-1} + 9S^2_{-1}S_1 + 12S_{-1}S^2_1 + 3S^3_1)] \\ & - \frac{\beta^4\tau}{192} [3S^3_{-1}S^2_1 + 3S_{-1}S^4_1 - 2B^4S_1 - B^2(3S^2_{-1}S_1 + 3S^3_1)] \\ & + \frac{\beta^3\tau^2}{192} [S^3_{-1}S^2_1 + 3S_{-1}S^4_1 + B^4S_{-1} \\ & + B^2(-2S^2_{-1}S_1 + 2S_{-1}S^2_1)]\end{aligned}$$

$$+\left(\frac{\beta^2\tau^3}{96}-\frac{\beta\tau^4}{192}\right)[2S_{-1}^3S_1^2-B^4(S_{-1}+2S_1)$$

$$-B^2(S_{-1}^2S_1+2S_{-1}S_1^2+3S_1^3)], \tag{5.16}$$

$$\langle \varrho S_1^x(\tau)\,S_1^x\rangle = \tfrac{1}{4}-\frac{(\beta\tau-\tau^2)}{8}(B^2+2S_1^2)$$

$$+\frac{\beta^3\tau}{96}[4S_{-1}^2S_1^2+2S_1^4+B^4+B^2(2S_{-1}^2+4S_{-1}S_1+6S_1^2)]$$

$$+\frac{\beta^2\tau^2}{16}S_1^4+\left(\frac{\tau^4}{96}-\frac{\beta\tau^3}{48}\right)$$

$$\times[4S_{-1}^2S_1^2+8S_1^4+B^4+B^2(2S_{-1}^2+4S_{-1}S_1+6S_1^2)]. \tag{5.17}$$

With the correlation functions (5.10) and (5.12)–(5.17) we can calculate the transverse susceptibility (3.9) per particle in the thermodynamic limit. The result is

$$\chi_{xx} = \tfrac{1}{4}\beta-\tfrac{1}{4}\beta^2S_{-1}+\frac{\beta^3}{48}(6S_{-1}^2-2S_1^2-B^2)$$

$$+\frac{\beta^4}{48}(-2S_{-1}^3+3S_{-1}S_1^2+2B^2S_{-1})$$

$$+\frac{\beta^5}{480}[5S_{-1}^4-16S_{-1}^2S_1^2+3S_1^4$$

$$+B^4+B^2(-13S_{-1}^2+4S_{-1}S_1+6S_1^2)]$$

$$+\frac{\beta^6}{2880}[-6S_{-1}^5+22S_{-1}^3S_1^2-33S_{-1}S_1^4$$

$$-17B^4S_{-1}+B^2(24S_{-1}^3-38S_{-1}^2S_1-70S_{-1}S_1^2)]. \tag{5.18}$$

Remarks. The *yy* component of the susceptibility tensor χ_{yy} can be obtained from the expression for χ_{xx} by the substitution $\gamma \to -\gamma$, which is equivalent to the interchange of S_{-1} and S_1.

The off-diagonal components χ_{xy}, χ_{xz} and χ_{yz} of the susceptibility tensor are equal to zero. For χ_{xz} and χ_{yz} this is easily appreciated, since the quantum-mechanical traces involved contain an odd number of α and β operators. For χ_{xy} one can easily check that all terms in the high-temperature expansions for the correlation functions are purely imaginary, and therefore cannot contribute to χ_{xy}.

6. *Results and conclusions.* In this section we shall give a few graphs of the transverse susceptibility χ_{xx} *vs.* one of the parameters β, γ of B (keeping the other two parameters fixed), and discuss some salient features*.

In fig. 1 the susceptibility is plotted *vs.* the inverse temperature β for various values of γ, keeping B fixed at $B = 0$.

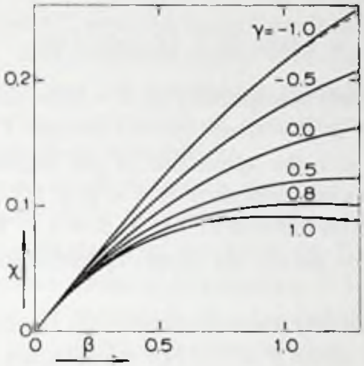

Fig. 1. The transverse susceptibility χ *vs.* the inverse temperature β in the absence of an external field B for various values of the anisotropy parameter γ. The dashed curves represent the exact expressions (6.1) and (6.2).

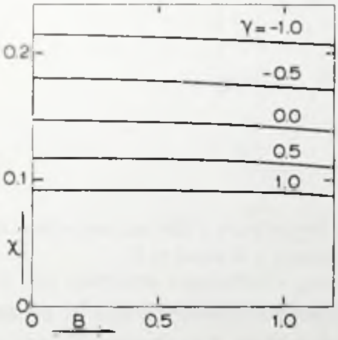

Fig. 2

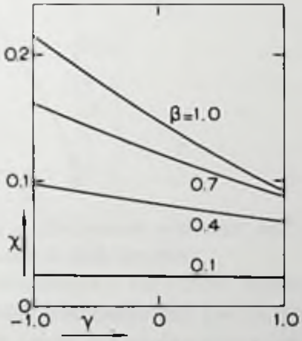

Fig. 3

Fig. 2. The transverse susceptibility χ *vs.* the external field B at $\beta = 1$ for various values of the anisotropy parameter γ.

Fig. 3. The transverse susceptibility χ *vs.* the anisotropy parameter γ in the absence of an external field B for various values of the inverse temperature β.

---

[*] Although the calculations given in this paper hold for arbitrary values of γ, we shall, when interpreting the results, restrict ourselves to the interval $-1 \leq \gamma \leq 1$, *i.e.* the antiferromagnetic XY chain.

The drawn curves have been obtained by using the high-temperature expansion up to β^6, the dashed curves represent the exact expressions for χ_{xx} at $\gamma = -1$ (the upper dashed curve) and at $\gamma = 1$ (the lower dashed curve) in the thermodynamic limit. These exact expressions are

$$\chi_{xx}\,(\gamma = 1, B = 0) = \tfrac{1}{4}\beta\, \mathrm{e}^{-\beta} \tag{6.1}$$

and

$$\chi_{xx}\,(\gamma = -1, B = 0) = \tfrac{1}{4}\tanh\tfrac{1}{2}\beta + \tfrac{1}{8}\beta\cosh^{-2}\tfrac{1}{2}\beta. \tag{6.2}$$

Eq. (6.1) is the (longitudinal) susceptibility at $B = 0$ for the Ising model. Eq. (6.2) can be obtained from χ_{zz} at $B = 0$ and $|\gamma| = 1$ for the XY model, by using *e.g.* eq. (39) of ref. 4. For $\beta \leq 1$ the agreement of the high-temperature expansion with the exact expressions is excellent. For $1 < \beta \leq 1.3$ there is a slight discrepancy which increases to an amount of 2% at $\beta = 1.3$. We note that for $\gamma = 1$ there is a maximum at $\beta = 1.0$ for the exact expression as well as for the expansion.

For $\gamma = 0.8$ the susceptibility reaches its maximum at about $\beta = 1.1$. For $\gamma = 0.5$ the maximum is found at about $\beta = 1.3$. For lower values of γ the maximum will occur at higher values of β.

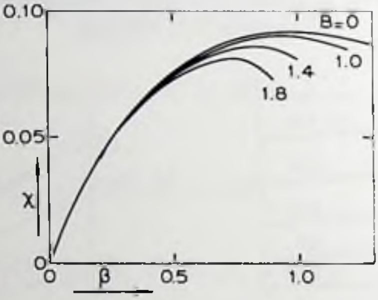

Fig. 4. The transverse susceptibility χ *vs.* the inverse temperature β for various values of the external field B; the anisotropy parameter γ is equal to 1.

For $\gamma = -1$ the value of β for which χ reaches its maximum can be estimated from the exact expression (6.2). This value is $\beta = 2.40$. The curves of fig. 1 refer to the case $B = 0$. A change of the magnetic field in the range $0 \leq B \leq 1.2$ would modify the picture only slightly.

This is shown in fig. 2, where we plot χ *vs.* B for various values of γ, β being fixed at $\beta = 1$. The variation in the range $0 \leq B \leq 1.2$ is at most 6%, and for lower values of β the variation is even smaller.

The dependence of χ on the anisotropy parameter γ, however, is very strong, *e.g.* at $\beta = 1$ and $B = 0$ the susceptibility for $\gamma = -1$ is 2.3 times as large as the susceptibility for $\gamma = 1$. This strong dependence is shown in fig. 3, where χ is plotted *vs.* γ for various values of β, keeping $B = 0$. Note that the steepness of the curves is the more pronounced as β increases. It is of interest to compare these dependences (weak on B, strong on γ) with the behaviour of the longitudinal susceptibility χ_{zz}. To this end we have estimated χ_{zz} for various values of γ, β and B, by using a high-temperature expansion of eq. (39) of ref. 4 up to β^7.

Firstly, we note that χ_{zz} does not depend on the sign of γ. But apart from this, it appears that for $\beta = 1$ and $0 \leq B \leq 1$ the longitudinal susceptibility χ_{zz} decreases only by at most 4% when $|\gamma|$ varies from 0 to 1; this change is even less for lower values of β. This contrasts clearly with the dependence of χ_{xx} on γ (see fig. 3). It is obvious that for establishing the anisotropy parameter of an XY system, the transverse susceptibility is a much more useful quantity to be measured than the longitudinal susceptibility.

As for the dependence on B, it appears that at $\beta = 1$ the longitudinal susceptibility χ_{zz} decreases by about 20%, when B varies from 0 to 1. This contrasts with the very weak dependence of χ_{xx} on B (see fig. 2). Finally, in figs. 4 and 5, we plot χ_{xx} *vs.* β for various values of B, keeping $\gamma = 1$ and $\gamma = 0.5$ respectively. One should realize that for the values $B = 1.4$ and $B = 1.8$ the expansion we have used, starts to be less reliable at β values of about 0.9.

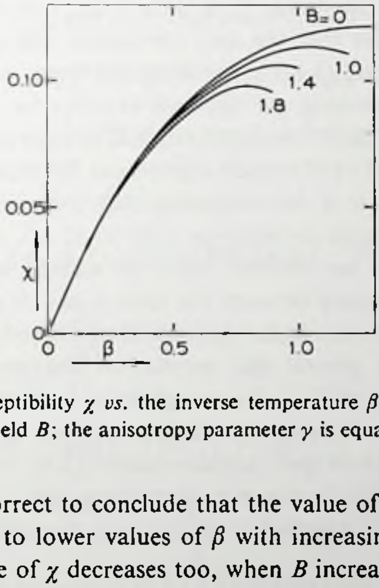

Fig. 5. The transverse susceptibility χ *vs.* the inverse temperature β for various values of the external field B; the anisotropy parameter γ is equal to 0.5.

It seems, however, correct to conclude that the value of β for which χ reaches its maximum decreases to lower values of β with increasing B, and furthermore that the maximum value of χ decreases too, when B increases.

7. *The susceptibility in the c-cyclic XY model.* In this section we shall investigate the susceptibility for the c-cyclic XY model, *i.e.*,

$$\chi = \lim_{N\to\infty} (1/N) \sum_{j,k=1}^{N} \langle \varrho_\sigma \int_0^\beta \mathrm{d}\tau\, S_j^x(\tau, \sigma)\, S_k^x \rangle, \tag{7.1}$$

where ϱ_σ, *cf.* (3.11), for $\sigma = -1, +1$ is the density operator corresponding to the c-cyclic and c-anticyclic hamiltonian $\mathscr{H}_\sigma$, given by eq. (2.23).

We shall show that the susceptibility (7.1) is different from the xx susceptibility (3.2) in the a-cyclic XY model, even in the thermodynamic limit.

From the KMS property (3.7) it follows that

$$\chi = \int_0^\beta \mathrm{d}\tau \lim_{N\to\infty} (1/N) \left(\sum_{j=1}^{N} \langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_j^x \rangle \right.$$

$$\left. + 2 \sum_{j=1}^{N} \sum_{p=1,2,\dots,N-j} \langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_{j+p}^x \rangle \right). \tag{7.2}$$

In contradistinction to the a-cyclic XY model, that is periodic in the spin components S^x, *cf.* eq. (2.2), we cannot restrict ourselves to the first spin with $j = 1$. In fact the spin correlation functions appearing in the right-hand side of (7.3) depend on j.

In the case that $j = 1$, the result is simple. Noting that the terms involving P can be omitted in the thermodynamic limit, *cf.* the discussion below eq. (4.4), and also noting that the factor $\sum_\sigma Z_\sigma/(Z_1 + Z_{-1})$ in eq. (4.5) can be omitted due to eq. (4.6), we see that the spin correlation functions $\langle \varrho_\sigma S_1^x(\tau,\sigma)\, S_{p+1}^x \rangle$, can be obtained from eq. (3.12) by omitting the factor $\exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})$, or equivalently, by replacing the operator $\exp \mathscr{L}_\sigma \tau$ by 1, *cf.* (4.14) and (4.15). Hence the correlation functions $\langle \varrho_\sigma S_1^x(\tau,\sigma)\, S_{p+1}^x \rangle$ are given by the coefficients A_p, defined by eq. (5.11) and explicit expressions for these coefficients have been listed in appendix E. It is not surprising that these correlation functions are different from the a-cyclic correlations $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$. In fact the c-cyclic and c-anticyclic model can be obtained from the a-cyclic model by introducing a disturbance in the coupling between the spins 1 and N and here we investigate the correlation function just at the position of the disturbance.

We now consider a general spin correlation function $\langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_{j+p}^x \rangle$, for sufficiently large values of j, *i.e.* far enough away from the disturbance by virtue of which the c-cyclic and c-anticyclic model have been introduced.

By using the Jordan–Wigner transformation (2.4), or more specifically the explicit expressions (2.30) for the spin components, and also the anticommutation relations (2.22), the spin correlation function can be written

$$\langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_{j+p}^x \rangle$$

$$= \tfrac{1}{2} \langle \varrho_\sigma \alpha_j(\tau,\sigma)\, (P_1 \cdots P_{j-1})(\tau,\sigma)\, P_1 \cdots P_{j-1} P_j \cdots P_{j+p-1} \alpha_{j+p} \rangle, \tag{7.3}$$

where $P_k = (2/\mathrm{i})\, \alpha_k \beta_k$. [Note that the factor $(P_1 \cdots P_{j-1})(\tau,\sigma)$ does not occur for $j = 1$, *cf.* eq. (7.9).]

In order to evaluate the right-hand side of (7.3), we use the identity

$$P_1 \cdots P_{j-1}\mathscr{H}_\sigma = (\mathscr{H}_\sigma - \sigma h + h_j)\, P_1 \cdots P_{j-1}, \tag{7.4}$$

where

$$h_j \equiv -2\mathrm{i}\,(S_{-1}\alpha_j\beta_{j-1} + S_1\alpha_{j-1}\beta_j). \tag{7.5}$$

Here h has been defined by eq. (2.8), *cf.* also eq. (4.20) and S_{-1} and S_1 have been given by eq. (4.23). The derivation of (7.4) is given in appendix G. From (7.4) it follows that

$$P_1 \cdots P_{j-1} \exp(-\tau\mathscr{H}_\sigma) = \exp[-\tau(\mathscr{H}_{-\sigma} + h_j)]\, P_1 \cdots P_{j-1}, \tag{7.6}$$

where also use has been made of the relation (4.1).

We now use (7.6), the trivial relations $P_j^2 = 1$ and the fact that the operators P_k commute among each other. Then the spin correlation function $\langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_{j+p}^x\rangle$ for $j > 1$, $j + p \leq N$ is given by

$$\begin{aligned}
\langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_{j+p}^x\rangle &= \tfrac{1}{2}\langle \varrho_\sigma \exp(\tau\mathscr{H}_\sigma)\,\alpha_j P_1 \cdots P_{j-1}\exp(-\tau\mathscr{H}_\sigma) \\
&\qquad \times P_1 \cdots P_{j-1} P_j \cdots P_{j+p-1}\alpha_{j+p}\rangle \\
&= \tfrac{1}{2}\langle \varrho_\sigma \exp(\tau\mathscr{H}_\sigma)\,\alpha_j \exp[-\tau(\mathscr{H}_{-\sigma} + h_j)] \\
&\qquad \times P_j \cdots P_{j+p-1}\alpha_{j+p}\rangle \\
&= \tfrac{1}{2}\langle \varrho_\sigma\alpha_j(\tau,\sigma)\exp(\tau\mathscr{H}_\sigma)\exp(-\tau\mathscr{H}_{-\sigma})\, O_j(\tau,-\sigma) \\
&\qquad \times \left(\prod_{k=j}^{j+p-1} (2/\mathrm{i})\,\alpha_k\beta_k\right)\alpha_{j+p}\rangle,
\end{aligned} \tag{7.7}$$

where

$$O_j(\tau,-\sigma) \equiv \exp(\tau\mathscr{H}_{-\sigma})\exp[-\tau(\mathscr{H}_{-\sigma} + h_j)]. \tag{7.8}$$

Eq. (7.8) is not valid for $j = 1$; we then have

$$\langle \varrho_\sigma S_1^x(\tau,\sigma)\, S_{p+1}^x\rangle = \tfrac{1}{2}\langle \varrho_\sigma\alpha_1(\tau,\sigma)\left(\prod_{k=1}^{p}(2/\mathrm{i})\,\alpha_k\beta_k\right)\alpha_{p+1}\rangle \tag{7.9}$$

For $O_j(\tau,-\sigma)$ we have the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}\tau} O_j(\tau,-\sigma) = [\mathscr{H}_{-\sigma}, O_j(\tau,-\sigma)] - O_j(\tau,-\sigma)\, h_j \tag{7.10}$$

and the formal solution can be written as

$$O_J(\tau, -\sigma) = \exp(\mathscr{L}_{-\sigma,J}\tau), \tag{7.11}$$

where the "Liouville operator" $\mathscr{L}_{-\sigma,J}$ is defined by its action on an arbitrary operator A, *i.e.*

$$\mathscr{L}_{-\sigma,J}A \equiv [\mathscr{H}_{-\sigma}, A] - Ah_J. \tag{7.12}$$

In particular, we have

$$\mathscr{L}_{-\sigma,J} = -h_J, \tag{7.13a}$$

$$\mathscr{L}^2_{-\sigma,J} = -[\mathscr{H}_{-\sigma}, h_J] + h_J^2. \tag{7.13b}$$

From (7.7), (7.11), (4.14) and (4.16) we have the expression

$$\langle \varrho_\sigma S_J^x(\tau, \sigma)\, S_{J+p}^x \rangle = \tfrac{1}{2} \langle \varrho_\sigma \alpha_J(\tau, \sigma) \times \exp(\mathscr{L}_\sigma \tau) \exp(\mathscr{L}_{-\sigma,J}\tau) \left(\prod_{k=J}^{J+p-1} (2/\mathrm{i})\, \alpha_k \beta_k \right) \alpha_{J+p} \rangle. \tag{7.14}$$

In order to evaluate the right-hand side let us first consider the correlation function $\langle \varrho S_J^x(\tau)\, S_{J+p}^x \rangle$ in the a-cyclic model. (Because of the translational invariance, this correlation function is of course equal to $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$.)

Using similar considerations as in the derivation of eqs. (3.12), (3.13) and (7.3), the correlation function can be written as

$$\langle \varrho S_J^x(\tau)\, S_{J+p}^x \rangle = \Big(\sum_\sigma Z_\sigma \langle \varrho_\sigma (1 + \sigma P) \rangle \Big)^{-1} \tfrac{1}{2} \sum_\sigma Z_\sigma \times \langle \varrho_\sigma \alpha_J(\tau, \sigma)\, (P_1 \cdots P_{J-1})\,(\tau, \sigma) \exp(\tau \mathscr{H}_\sigma) \exp(-\tau \mathscr{H}_{-\sigma})\, P_1 \cdots P_{J-1} P_J \cdots P_{J+p-1} \alpha_{J+p} (1 + \sigma P) \rangle. \tag{7.15}$$

Using eq. (7.6) with $-\sigma$ instead of σ and using a similar line of reasoning as in the derivation of eqs. (7.7) and (7.14), it can be shown that

$$\langle \varrho S_J^x(\tau)\, S_{J+p}^x \rangle \Big(\sum_\sigma Z_\sigma \langle \varrho_\sigma (1 + \sigma P) \rangle \Big)$$

$$= \tfrac{1}{2} \sum_\sigma Z_\sigma \langle \varrho_\sigma \exp(\tau \mathscr{H}_\sigma)\, \alpha_J P_1 \cdots P_{J-1} \exp(-\tau \mathscr{H}_{-\sigma}) \times P_1 \cdots P_{J-1} P_J \cdots P_{J+p-1} \alpha_{J+p} (1 + \sigma P) \rangle$$

$$= \tfrac{1}{2} \sum_\sigma Z_\sigma \langle \varrho_\sigma \alpha_J(\tau, \sigma) \exp(\tau \mathscr{H}_\sigma) \exp[-\tau(\mathscr{H}_\sigma + h_J)]$$

$$\times\, P_j \cdots P_{j+p-1}\alpha_{j+p}(1+\sigma P)\rangle$$

$$= \tfrac{1}{2}\sum_{\sigma} Z_{\sigma}\, \langle \varrho_{\sigma}\alpha_j(\tau,\sigma)\, O_j(\tau,\sigma)\, P_j \cdots P_{j+p-1}\alpha_{j+p}(1+\sigma P)\rangle$$

$$= \tfrac{1}{2}\sum_{\sigma} Z_{\sigma}\, \langle \varrho_{\sigma}\alpha_j(\tau,\sigma)\exp(\mathscr{L}_{\sigma,j}\tau)\left(\prod_{k=j}^{j+p-1}(2/\mathrm{i})\,\alpha_k\beta_k\right)\alpha_{j+p}(1+\sigma P)\rangle. \tag{7.16}$$

In the same way as we did in section 4 it can be argued that the terms involving the operator P can be omitted in the thermodynamic limit for non-zero temperatures and furthermore the average $\langle \varrho_{\sigma} \cdots\rangle$ occurring in the right-hand side of (7.16) can be seen to be independent of σ, *cf.* the discussions below eqs. (4.5), (4.6) and (4.17). The a-cyclic correlation function is then given by

$$\langle \varrho S_j^x(\tau)\, S_{j+p}^x\rangle$$
$$= \tfrac{1}{2}\langle \varrho_{\sigma}\alpha_j(\tau,\sigma)\exp(\mathscr{L}_{\sigma,j}\tau)\left(\prod_{k=j}^{j+p-1}(2/\mathrm{i})\,\alpha_k\beta_k\right)\alpha_{j+p}\rangle. \tag{7.17}$$

Eq. (7.17) obviously is equal to the correlation function $\langle \varrho S_1^x(\tau)\, S_{p+1}^x\rangle$ given by eq. (4.17). First of all the right-hand sides of (7.17) and (4.17) are independent of σ, so that we can restrict ourselves to the c-cyclic case with $\sigma = -1$. If we then apply the translation $\mathscr{T}$ over $j-1$ lattice sites which transforms in particular the pair of neighbours $j-1, j$ into the pair of neighbours N, 1, the operator $\exp(\mathscr{L}_{-1,j}\tau)$, defined by (7.11) and (7.8) for $\sigma = 1$, is transformed into the operator

$$\mathscr{T}\exp(\mathscr{L}_{-1,j}\tau)\,\mathscr{T}^{-1} = \exp(\tau\mathscr{H}_{-1})\exp[-\tau(\mathscr{H}_{-1}+h)]$$
$$= \exp(\tau\mathscr{H}_{-1})\exp(-\tau\mathscr{H}_{1}) = \exp(\mathscr{L}_{-1}\tau), \tag{7.18}$$

so that the translational invariance is shown in an explicit way by (7.17).

If we now compare the second line of the right-hand side of eq. (7.7) with the second line on the right-hand side of eq. (7.16), we see that the operator $\exp[-\tau(\mathscr{H}_{-\sigma}+h_j)]$ occurring in eq. (7.7) for the c-cyclic correlation function has been replaced by the factor $\exp[-\tau(\mathscr{H}_{\sigma}+h_j)]$ occurring in eq. (7.16) for the a-cyclic correlation function. This replacement is a direct consequence of the commutation relation (2.37) for S_j^x, which involves both projection operators P_{σ} and $P_{-\sigma}$.

As a result the c-cyclic correlation function $\langle \varrho_{\sigma} S_j^x(\tau,\sigma)\, S_{j+p}^x\rangle$ given by eq. (7.14) for $j \neq 1$ contains an additional operator $\exp \mathscr{L}_{\sigma}\tau$, which does not occur in the corresponding expression eq. (7.17) for the a-cyclic correlation function. We now consider eq. (7.14). Assuming that the correlation function (7.14) can be expanded as a power series in τ and β, we have for sufficiently large values of j and $N - j$, $(j + p \leq N)$, the decoupling

$$\langle \varrho_\sigma S_j^x(\tau, \sigma)\, S_{j+p}^x \rangle = \tfrac{1}{2}\langle \varrho_\sigma \exp(\mathscr{L}_\sigma \tau)\rangle$$
$$\times \langle \varrho_\sigma \alpha_j(\tau, \sigma) \exp(\mathscr{L}_{-\sigma, j}\tau) \left(\prod_{k=j}^{j+p-1} (2/\mathrm{i})\, \alpha_k \beta_k \right) \alpha_{j+p} \rangle . \tag{7.19}$$

Eq. (7.19) is proved in more detail in appendix H. In addition, for sufficiently large values of j, if we restrict ourselves to contributions $\approx \tau^\mu \beta^\lambda$ satisfying $\lambda + \mu \leq \nu - 1$, *cf.* (4.12), the operator $\exp(+\mathscr{L}_{-\sigma, j}\tau)$ on the right-hand side of (7.19) can be replaced by $\exp(+\mathscr{L}_{\sigma, j}\tau)$ and due to of (7.17), we have the simple relation

$$\langle \varrho_\sigma S_j^x(\tau, \sigma)\, S_{j+p}^x \rangle = \langle \varrho_\sigma \exp(\mathscr{L}_\sigma \tau)\rangle \langle \varrho S_j^x(\tau)\, S_{j+p}^x \rangle \tag{7.20}$$

for sufficiently large values of j and $N - j$. Hence the correlation function in the c-cyclic model can be obtained from those in the a-cyclic model after multiplication by the factor $\langle \varrho_\sigma \exp \mathscr{L}_\sigma \tau \rangle$. The evaluation of this factor is straightforward. If we restrict ourselves to the case that $\nu = 4$, "the relevant part" of $\exp \mathscr{L}_{-1}\tau$, *i.e.*, the terms which give contributions $\approx \tau^\mu \beta^\lambda$ with $\lambda + \mu \leq 3$, is given by

$$\exp(\mathscr{L}_{-1}\tau) = 1 + 2\mathrm{i}\tau(S_{-1}\alpha_1\beta_N + S_1\alpha_N\beta_1) + \tfrac{1}{2}1\tau^2(S_{-1}^2 + S_1^2), \tag{7.21}$$

so that

$$\langle \varrho_{-1} \exp(\mathscr{L}_{-1}\tau)\rangle = 1 + \tfrac{1}{2}(\tau^2 - \beta\tau)(S_{-1}^2 + S_1^2). \tag{7.22}$$

Using eqs. (7.20), (7.22) and the a-cyclic correlation functions (5.16) and (5.17), the c-cyclic susceptibility (7.3) up to order β^4 is given by

$$\chi_{\text{c-cyclic}} = \chi_{\text{a-cyclic}} - (\beta^3/48)(S_{-1}^2 + S_1^2) + (\beta^4/48)\, S_{-1}(S_{-1}^2 + S_1^2). \tag{7.23}$$

Here $\chi_{\text{a-cyclic}}$ is the a-cyclic susceptibility given by eq. (5.18). The result is

$$\chi_{\text{c-cyclic}} = \tfrac{1}{4}\beta - \tfrac{1}{4}\beta^2 S_{-1} + (\beta^3/48)(5S_{-1}^2 - 3S_1^2 - B^2)$$
$$+ (\beta^4/48)(-S_{-1}^3 + 4S_{-1}S_1^2 + 2B^2 S_{-1}). \tag{7.24}$$

Hence, the c-cyclic model cannot be used to evaluate the xx susceptibility of the a-cyclic XY model, even in the thermodynamic limit. For arbitrarily large values of j, the effect of the local disturbance in the coupling between the spins 1 and N

on the correlation function $\langle \varrho_\sigma S_j^x(\tau, \sigma)\, S_{j+p}^x \rangle$ is not negligible. This is due to the fact that the Jordan–Wigner operators $P_1(\tau, \sigma) \cdots P_{j-1}(\tau, \sigma)$ in eq. (7.3) are "time dependent".

APPENDIX A

In this appendix we prove that the perturbation expansion (4.2) is convergent. Consider the contribution $C^{(q)}$ of the qth order of perturbation to the correlation function $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$. Noting that the terms with the operator P can be neglected in the thermodynamic limit and using the fact that the factor $\sum_\sigma Z_\sigma/(Z_1 + Z_{-1})$ in eq. (4.5) can be omitted, *cf.* (4.6), $C^{(q)}$ can be written

$$C^{(q)} = \tfrac{1}{2} \langle \exp(-\beta \mathscr{H}_\sigma) \rangle^{-1} \int_0^\tau \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \cdots \int_0^{\tau_{q-1}} \mathrm{d}\tau_q \sigma^q$$
$$\times \langle \mathrm{e}^{-(\beta-\tau)\mathscr{H}_\sigma} \alpha_1\, \mathrm{e}^{-(\tau-\tau_1)\mathscr{H}_\sigma} h\, \mathrm{e}^{-(\tau_1-\tau_2)\mathscr{H}_\sigma} h \cdots \mathrm{e}^{-(\tau_{q-1}-\tau_q)\mathscr{H}_\sigma} h\, \mathrm{e}^{-\tau_q \mathscr{H}_\sigma} B \rangle, \tag{A.1}$$

where

$$B \equiv \left(\prod_{j=1}^{p} (2/\mathrm{i})\, \alpha_j \beta_j \right) \alpha_{p+1}. \tag{A.2}$$

In order to estimate $C^{(q)}$, we use the Hölder inequality for operators

$$|\langle O_1 O_2 \cdots O_n \rangle| \le \prod_{k=1}^{n} \langle (O_k^\dagger O_k)^{\frac{1}{2}\theta_k} \rangle^{1/\theta_k}, \tag{A.3}$$

for arbitrary operators O_k and nonnegative numbers $\theta_1, \theta_2, \ldots, \theta_n$ satisfying

$$\sum_{k=1}^{n} \theta_k^{-1} = 1. \tag{A.4}$$

A simple proof of this inequality was given in ref. 14. For arbitrary real positive numbers $\lambda_1, \lambda_2, \ldots, \lambda_s$ with

$$\lambda_1 + \lambda_2 + \cdots + \lambda_s = \beta \tag{A.5}$$

and a hermitean operator O, we have in particular the inequality

$$\langle \mathrm{e}^{-\beta O} \rangle^{-1} |\langle \mathrm{e}^{-\lambda_1 O} O_1\, \mathrm{e}^{-\lambda_2 O} O_2 \cdots \mathrm{e}^{-\lambda_s O} O_s \rangle| \le \|O_1\|\, \|O_2\| \cdots \|O_s\|, \tag{A.6}$$

where $\|O_k\|$ is the norm of the operator O_k, *i.e.* the largest eigenvalue of $(O_k^\dagger O_k)^{\frac{1}{2}}$. Eq. (A.6) follows immediately from (A.3) by choosing

$$\begin{aligned} &n = 2s, \qquad \theta_2^{-1} = \theta_4^{-1} = \cdots = \theta_{2s}^{-1} = 0, \\ &\theta_1 = \beta/\lambda_1, \qquad \theta_3 = \beta/\lambda_2, \ldots, \theta_{2s-1} = \beta/\lambda_s. \end{aligned} \tag{A.7}$$

The simple version (A.6) of the Hölder inequality has been applied previously by Ginibre and Gruber[15]).

From (A.1) and (A.6) it is now obvious that

$$|C^{(q)}| \leq \tfrac{1}{2}\,(\beta^q/q!)\, \|\alpha_1\|\; \|h\|^q\; \|B\| \tag{A.8}$$

and all the operator norms on the right-hand side of (A.8) are finite.

APPENDIX B

In this appendix we give the expression for the operator $\mathscr{L}_\sigma^3$, where $\mathscr{L}_\sigma$ is defined by eq. (4.13). It is given by

$$\begin{aligned}\mathscr{L}_\sigma^3 = (-2\mathrm{i}\sigma)\,\{&6\sigma S_1 S_{-1}^2\,(\alpha_1\beta_1\beta_{N-1}\beta_N - \alpha_1\alpha_2\alpha_N\beta_N)\\ &+ 6\sigma S_{-1}S_1^2\,(\beta_1\beta_2\beta_N\alpha_N - \beta_1\alpha_1\alpha_{N-1}\alpha_N)\\ &+ \alpha_1\beta_N\,[S_{-1}^3 + 5S_{-1}S_1^2 + 2B^2\,(S_{-1} - S_1)]\\ &+ \alpha_N\beta_1\,[S_1^3 + 5S_{-1}^2S_1 + 2B^2\,(S_1 - S_{-1})]\\ &- BS_{-1}\,(S_{-1} - S_1)\,(\alpha_2\beta_N + \alpha_1\beta_{N-1})\\ &- BS_1\,(S_1 - S_{-1})\,(\alpha_N\beta_2 + \alpha_{N-1}\beta_1) + \alpha_3\beta_N S_{-1}^2 S_1 + \alpha_N\beta_3 S_1^2 S_{-1}\\ &- 2\alpha_2\beta_{N-1}S_{-1}^2S_1 - 2\alpha_{N-1}\beta_2 S_{-1}S_1^2\}.\end{aligned} \tag{B.1}$$

APPENDIX C

In this appendix we prove eq. (4.26) by induction over n. Suppose it is true for $\mathscr{L}_\sigma^n$, then each term in the right-hand side of eq. (4.24) contains $\frac{1}{2}\,(k + l)$ operators with an index $\mathcal{O}(1)$ and $\frac{1}{2}\,(k + l)$ operators with an index $\mathcal{O}(N)$. In order to prove (4.26) for $\mathscr{L}_\sigma^{n+1}$ we first note that the commutation with $\mathscr{H}_\sigma$ does not change the number of different operators α and β, *i.e.* if we take from (4.24) a term T with $k + l$ different operators, then $[\mathscr{H}_\sigma, T]$ has also $k + l$ different operators. Suppose $[\mathscr{H}_\sigma, T]$ has a term with $k + l - 2$ different operators. This can occur at least in principle, if in the term $T = \alpha_{l_1}\alpha_{l_2}\cdots\alpha_{l_k}\beta_{J_1}\cdots\beta_{J_l}$, we have operators α_{l_p} and β_{J_q} such that

$$[\mathscr{H}_\sigma, \alpha_{l_p}] = -\mathrm{i}(S_\sigma)_{l_pJ_q}\,\beta_{J_q} + \text{other terms}, \qquad (S_\sigma)_{l_pJ_q} \neq 0, \tag{C.1}$$

then we have two operators β_{J_q} after the commutation and these two operators can be eliminated using the anticommutation relations. However, in that case we can write

$$T = A\alpha_{i_p}\beta_{j_q}, \tag{C.2}$$

where A is an operator which does not contain α_{i_p} and β_{j_q}. Then

$$[\mathscr{H}_\sigma, T] = [\mathscr{H}_\sigma, A]\,\alpha_{i_p}\beta_{j_q} + A\,[\mathscr{H}_\sigma, \alpha_{i_p}\beta_{j_q}], \tag{C.3}$$

where

$$\begin{aligned}[\mathscr{H}_\sigma, \alpha_{i_p}\beta_{j_q}] &= -\mathrm{i}\sum_k (\mathrm{S}_\sigma)_{i_p k}\,\beta_k\beta_{j_q} + \mathrm{i}\sum_k (\mathrm{S}_\sigma)_{k j_q}\,\alpha_{i_p}\alpha_k \\ &= -\mathrm{i}\sum_{k \neq j_q} (\mathrm{S}_\sigma)_{i_p k}\,\beta_k\beta_{j_q} + \mathrm{i}\sum_{k \neq i_p} (\mathrm{S}_\sigma)_{k j_q}\,\alpha_{i_p}\alpha_k \end{aligned} \tag{C.4}$$

and the right-hand side of (C.4) is a bilinear form in the operators α and β. Hence $[\mathscr{H}, T]$ contains $k + l$ different operators α and β. In view of the identity

$$[\mathscr{H}_\sigma, C_1C_2 \cdots C_s] = \sum_l C_1 \cdots C_{l-1}\,[\mathscr{H}_\sigma, C_l]\,C_{l+1} \cdots C_s, \tag{C.5}$$

$[\mathscr{H}_\sigma, T]$ contains at least $\frac{1}{2}(k + l) - 1$ operators with index $\mathcal{O}(N)$. Furthermore only terms T involving $\alpha_1, \alpha_N, \beta_1, \beta_N$ can lead to terms $[\mathscr{H}_\sigma, T]$ which have a number of operators with index $\mathcal{O}(N)$, which is different from $\frac{1}{2}(k + l)$. So we can restrict our attention to terms T, in which

$$i_1 = 1, \qquad \text{or} \qquad i_k = N, \qquad \text{or} \qquad j_1 = 1, \qquad \text{or} \qquad j_l = N. \tag{C.6}$$

Consider now the product $T\sigma h$. Only the terms which satisfy one of the four conditions

$$i_1 = 1,\ j_l \neq N;\ i_k = N,\ j_l \neq 1;\ i_l \neq 1,\ j_l = N;\ i_k \neq N,\ j_1 = 1, \tag{C.7}$$

can lead to terms in which the number of operators with index $\mathcal{O}(N)$ is different from the number of operators with index $\mathcal{O}(1)$. Using eqs. (C.6) and (C.7), we find

$$\begin{aligned}\mathscr{L}_\sigma^{n+1} = [\mathscr{H}_\sigma, \mathscr{L}_\sigma^n] + \mathscr{L}_\sigma^n\sigma h = \sum_{k,l} \sum_{\substack{i_1 < i_2 < \cdots < i_k \\ j_1 < j_2 < \cdots < j_l}} & C^{(n)}_{i_1 \cdots i_k; j_1 \cdots j_l} \\ \times \{ & -\mathrm{i}(\mathrm{S}_\sigma)_{1N}\,[\beta_N\alpha_{i_2} \cdots \alpha_{i_k}\beta_{j_1} \cdots \beta_{j_l}\delta_{i_1,1} - \alpha_{i_1} \cdots \alpha_{i_k}\beta_{j_1} \cdots \beta_{j_{l-1}}\alpha_1\,\delta_{j_l,N}] \\ & - \mathrm{i}(\mathrm{S}_\sigma)_{N1}\,[\alpha_{i_1} \cdots \alpha_{i_{k-1}}\beta_1\beta_{j_1} \cdots \beta_{j_l}\delta_{i_k,N} - \alpha_{i_1} \cdots \alpha_{i_k}\alpha_N\beta_{j_2} \cdots \beta_{j_l}\delta_{j_1,1}] \\ & - 2\mathrm{i}\sigma S_{-1}\,[\delta_{i_1,1}(1 - \delta_{j_l,N}) + \delta_{j_l,N}(1 - \delta_{i_1,1})]\,\alpha_{i_1} \cdots \alpha_{i_k}\beta_{j_1} \cdots \beta_{j_l}\alpha_1\beta_N \\ & - 2\mathrm{i}\sigma S_1\,[\delta_{i_k,N}(1 - \delta_{j_1,1}) + \delta_{j_1,1}(1 - \delta_{i_k,N})]\,\alpha_{i_1} \cdots \alpha_{i_k}\beta_{j_1} \cdots \beta_{j_l}\alpha_N\beta_1\} \\ & + \text{other terms.}\end{aligned} \tag{C.8}$$

Here the other terms contain the same number of operators with index $\mathcal{C}(1)$ as operators with index $\mathcal{C}(N)$. By using the commutation relations (2.22) and also the relations $(\mathrm{S}_\sigma)_{1N} = -\sigma S_{-1}$, $(\mathrm{S}_\sigma)_{N1} = -\sigma S_1$, *cf.* (2.24) and (2.25), it can be shown that the term between curly brackets in the right-hand side of (C.8) vanishes, so that

$$\mathscr{L}_\sigma^{n+1} = \text{other terms}, \tag{C.9}$$

i.e., each term of $\mathscr{L}_\sigma^{n+1}$ contains as many operators with index $\mathcal{C}(1)$ as operators with index $\mathcal{O}(N)$.

APPENDIX D

In this appendix we give some matrix elements $(\mathrm{M}_\sigma)_q \equiv (\mathrm{M}_\sigma)_{k,\,k+q}$, $(\mathrm{S}_\sigma \mathrm{M}_\sigma)_q$, $(\mathrm{M}_\sigma^2)_q$ and $(\mathrm{S}_\sigma \mathrm{M}_\sigma^2)_q$ for small values of $|q|$. These matrix elements are independent of σ and have been used in the calculation of the spin correlation functions in section 5.

$$M_0 = S_{-1}^2 + S_1^2 + B^2, \tag{D.1}$$

$$M_1 = M_{-1} = -B(S_{-1} + S_1), \qquad M_2 = M_{-2} = S_{-1}S_1, \tag{D.2}$$

$$(\mathrm{SM})_2 = -B(S_1^2 + 2S_{-1}S_1), \tag{D.3}$$

$$(\mathrm{SM})_1 = 2S_{-1}^2 S_1 + S_1^3 + B^2(S_{-1} + 2S_1), \tag{D.4}$$

$$(\mathrm{SM})_0 = -B^3 - 2B(S_{-1}^2 + S_{-1}S_1 + S_1^2), \tag{D.5}$$

$$(\mathrm{SM})_{-1} = S_{-1}^3 + 2S_{-1}S_1^2 + B^2(2S_{-1} + S_1), \tag{D.6}$$

$$(\mathrm{SM})_{-2} = -B(S_{-1}^2 + 2S_{-1}S_1), \tag{D.7}$$

$$(\mathrm{M}^2)_1 = -2\,[B^3(S_{-1} + S_1) + B(S_{-1}^3 + 2S_{-1}^2 S_1 + 2S_{-1}S_1^2 + S_1^3)], \tag{D.8}$$

$$(\mathrm{M}^2)_0 = S_{-1}^4 + 4S_{-1}^2 S_1^2 + S_1^4 + B^4 + 4B^2(S_{-1}^2 + S_{-1}S_1 + S_1^2), \tag{D.9}$$

$$\begin{aligned}(\mathrm{SM}^2)_{-1} = {} & S_{-1}^5 + 6S_{-1}^3 S_1^2 + 3S_{-1}S_1^4 + B^4(3S_{-1} + 2S_1) \\ & + 3B^2(2S_{-1}^3 + 3S_{-1}^2 S_1 + 4S_{-1}S_1^2 + S_1^3).\end{aligned} \tag{D.10}$$

APPENDIX E

In this appendix we give explicit expressions for the contribution A_p to the spin correlation functions $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$ arising from the term 1 in eq. (5.3). We have

$$A_p = 0, \qquad p \geq 6, \tag{E.1}$$

$$A_5 = -\frac{\beta^5}{128} S_{-1}^5, \tag{E.2}$$

$$A_4 = \frac{\beta^4}{64} S_{-1}^4, \tag{E.3}$$

$$A_3 = -\frac{\beta^3}{32} S_{-1}^3 + \frac{\beta^5}{384} (3S_{-1}^5 + 5S_{-1}^3 S_1^2 + 4B^2 S_{-1}^3) + \frac{(\beta^4\tau - \beta^3\tau^2)}{64} S_{-1}^5, \tag{E.4}$$

$$A_2 = \frac{\beta^2}{16} S_{-1}^2 - \frac{\beta^4}{192} (2S_{-1}^4 + 4S_{-1}^2 S_1^2 + 3B^2 S_{-1}^2) - \frac{(\beta^3\tau - \beta^2\tau^2)}{32} S_{-1}^4, \tag{E.5}$$

$$\begin{aligned} A_1 = {} & -\frac{\beta}{8} S_{-1} + \frac{\beta^3}{96} [S_{-1}^3 + 2S_{-1} S_1^2 + B^2 (2S_{-1} + S_1)] \\ & + \frac{(\beta^2\tau - \beta\tau^2)}{16} (S_{-1}^3 + S_{-1} S_1^2 - B^2 S_1) \\ & - \frac{\beta^5}{960} [S_{-1}^5 + 6S_{-1}^3 S_1^2 + 3S_{-1} S_1^4 + B^4 (3S_{-1} + 2S_1) \\ & + B^2 (6S_{-1}^3 + 9S_{-1}^2 S_1 + 12S_{-1} S_1^2 + 3S_1^3)] \\ & - \frac{\beta^4\tau}{192} [2S_{-1}^5 + 7S_{-1}^3 S_1^2 + 3S_{-1} S_1^4 - 2B^4 S_1 + 3B^2 (S_{-1}^3 - S_{-1}^2 S_1 - S_1^3)] \\ & + \frac{\beta^3\tau^2}{192} [S_{-1}^5 + 3S_{-1}^3 S_1^2 + 2S_{-1} S_1^4 + B^4 S_{-1} + B^2 (S_{-1}^3 - 3S_{-1}^2 S_1 - S_1^3)] \\ & + \left(\frac{\beta^2\tau^3}{96} - \frac{\beta\tau^4}{192} \right) [S_{-1}^5 + 4S_{-1}^3 S_1^2 + S_{-1} S_1^4 \\ & - B^4 (S_{-1} + 2S_1) + 2B^2 (S_{-1}^3 - S_1^3)], \end{aligned} \tag{E.6}$$

$$\begin{aligned} A_0 = {} & \frac{1}{4} - \frac{(\beta\tau - \tau^2)}{8} (S_{-1}^2 + S_1^2 + B^2) + \left(\frac{\beta^3\tau}{96} - \frac{\beta\tau^3}{48} + \frac{\tau^4}{96} \right) \\ & \times [S_{-1}^4 + 4S_{-1}^2 S_1^2 + S_1^4 + B^4 + 4B^2 (S_{-1}^2 + S_{-1} S_1 + S_1^2)]. \end{aligned} \tag{E.7}$$

APPENDIX F

In this appendix we give explicit expressions for the contributions B_p to the spin correlation functions $\langle \varrho S_1^x(\tau)\, S_{p+1}^x \rangle$ arising from $\exp(\mathscr{L}_1\tau) - 1$ in eq. (5.3). We have

$$B_p = 0, \qquad \text{if} \qquad p \geq 4 \qquad (\text{also if } p \leq N-3), \tag{F.1}$$

$$B_3 = \frac{\beta^3\tau^2}{128}\left(-2c_0^{(2)}S_{-1}^3 + c_5^{(2)}S_{-1}^2S_1\right) - \left(\frac{\beta^4\tau}{64} - \frac{\beta^3\tau^2}{32}\right), \tag{F.2}$$

$$B_2 = \frac{\beta^2\tau^2}{64}\left(2c_0^{(2)}S_{-1}^2 - c_5^{(2)}S_{-1}S_1\right) + \left(\frac{\beta^3\tau}{32} - \frac{\beta^2\tau^2}{16}\right), \tag{F.3}$$

$$\begin{aligned}
B_1 = {} & \frac{\beta\tau^4}{768}\left(-4c_0^{(4)}S_{-1} + 2c_1^{(4)}S_1 + c_2^{(4)}B - c_3^{(4)}S_1\right) \\
& + \left(\frac{\beta\tau^4}{96} - \frac{\beta^2\tau^3}{192}\right)\left[2c_1^{(3)}S_{-1}^2 - c_6^{(3)}\left(S_{-1}S_1 - B^2\right)\right] \\
& + \frac{\beta^2\tau^3}{192}\left(2c_4^{(3)}BS_1 - 2c_5^{(3)}S_1^2 + c_7^{(3)}B^2\right) - \frac{\beta\tau^2}{16}\, c_0^{(2)}S_{-1} \\
& - \frac{\beta\tau^2}{32}\, c_5^{(2)}S_1 + \frac{\beta^3\tau^2}{384}\left\{2c_0^{(2)}\left[S_{-1}^3 + 2S_{-1}S_1^2 + B^2\left(2S_{-1} + S_1\right)\right]\right. \\
& + c_2^{(2)}B\left(S_{-1}^2 + 2S_{-1}S_1\right) - c_4^{(2)}S_{-1}^2S_1 \\
& \left. - c_5^{(2)}\left[2S_{-1}^2S_1 + S_1^3 + B^2\left(S_{-1} + 2S_1\right)\right]\right\} \\
& + \frac{\left(\beta^2\tau^3 - \beta\tau^4\right)}{128}\left[4c_0^{(2)}\left(S_{-1}^3 + S_{-1}S_1^2 - B^2S_1\right)\right. \\
& + 2c_1^{(2)}B\left(S_{-1}^2 - S_1^2\right) - 2c_2^{(2)}B\left(S_{-1}^2 + S_{-1}S_1\right) \\
& \left. - 2c_3^{(2)}S_{-1}^2S_1 - 2c_5^{(2)}\left(S_{-1}^2S_1 + S_1^3 - B^2S_{-1}\right) - c_7^{(2)}B^2\left(S_{-1} + S_1\right)\right] \\
& - \left(\frac{\beta^2\tau}{16} - \frac{\beta\tau^2}{8}\right)S_{-1}^3 + \frac{\beta^4\tau}{192}\left(2S_{-1}^5 + 4S_{-1}^3S_1^2 + 3B^2S_{-1}^3\right) \\
& + \frac{\beta^3\tau^2}{96}\, B^2\left(S_{-1}^3 - S_{-1}^2S_1\right) - \left(\frac{\beta^3\tau^2}{96} + \frac{\beta^2\tau^3}{32} - \frac{\beta\tau^4}{48}\right) \\
& \times \left(S_{-1}^5 + 2S_{-1}^3S_1^2 + 2B^2S_{-1}^3 + B^2S_{-1}^2S_1\right),
\end{aligned} \tag{F.4}$$

$$\begin{aligned} B_0 = {} & \frac{\tau^4}{96} c_0^{(4)} - \frac{\tau^4}{24} c_1^{(3)} S_{-1} + \frac{\beta\tau^3}{48} (c_1^{(3)} S_{-1} - c_2^{(3)} S_1) \\ & + \frac{\tau^2}{8} c_0^{(2)} + \left(\frac{\beta^2\tau^2}{128} - \frac{\beta\tau^3}{64}\right) c_7^{(2)} (S_{-1} S_1 - B^2) \\ & + \frac{(\beta\tau^3 - \tau^4)}{32} [-c_1^{(2)} B (S_{-1} + S_1) + c_3^{(2)} S_{-1} S_1 + c_0^{(2)} (S_{-1}^2 + S_1^2 + B^2)] \\ & + \frac{\beta\tau}{8} (S_{-1}^2 - S_1^2) - \frac{\tau^2}{4} S_{-1}^2 - \frac{\beta^3\tau}{96} (S_{-1}^4 - S_1^4 + 2B^2 S_{-1}^2 - 2B^2 S_1^2) \\ & + \frac{\beta^2\tau^2}{16} (S_1^4 + S_{-1}^2 S_1^2 - B^2 S_{-1} S_1) \\ & - \frac{\tau^4}{24} (S_{-1}^4 + 2S_{-1}^2 S_1^2 + 2B^2 S_{-1}^2 + B^2 S_{-1} S_1) \\ & + \frac{\beta\tau^3}{16} (S_{-1}^4 + S_{-1}^2 S_1^2 - S_1^4 + 2B^2 S_{-1}^2 + 2B^2 S_{-1} S_1). \end{aligned} \tag{F.5}$$

The contributions B_3, B_2, B_1, B_0 can be calculated using the explicit expressions (5.4), (5.5) and (5.6). The result is

$$B_3 = -\frac{(\beta^4\tau - \beta^3\tau^2)}{64} S_{-1}^5, \tag{F.6}$$

$$B_2 = \frac{(\beta^3\tau - \beta^2\tau^2)}{32} S_{-1}^4, \tag{F.7}$$

$$\begin{aligned} B_1 = {} & -\frac{(\beta^2\tau - \beta\tau^2)}{16} S_{-1}^3 + \frac{\beta^4\tau}{192} (2S_{-1}^5 + 4S_{-1}^3 S_1^2 + 3B^2 S_{-1}^3) \\ & - \frac{\beta^3\tau^2}{192} [S_{-1}^5 + 2S_{-1}^3 S_1^2 - S_{-1} S_1^4 + B^2 (S_{-1}^3 - S_{-1}^2 S_1 - 2S_{-1} S_1^2 - S_1^3)] \\ & - \left(\frac{\beta^2\tau^3}{96} - \frac{\beta\tau^4}{192}\right) [S_{-1}^5 + 2S_{-1}^3 S_1^2 + S_{-1} S_1^4 \\ & + B^2 (2S_{-1}^3 + S_{-1}^2 S_1 + 2S_{-1} S_1^2 + S_1^3)], \end{aligned} \tag{F.8}$$

$$B_0 = \tfrac{1}{8}(\beta\tau - \tau^2)(S_{-1}^2 - S_1^2) + \frac{\beta^3\tau}{96}[-S_{-1}^4 + S_1^4 - 2B^2(S_{-1}^2 - S_1^2)]$$

$$+ \frac{\beta^2\tau^2}{16} S_1^4 + \left(\frac{\beta\tau^3}{48} - \frac{\tau^4}{96}\right)[S_{-1}^4 - 7S_1^4 + 2B^2(S_{-1}^2 - S_1^2)]. \quad \text{(F.9)}$$

Note that the coefficients $c_6^{(2)}$ and $c_3^{(3)}$ do not occur explicitly in eqs. (F.1)–(F.5). The corresponding operators $\beta_2\beta_N$ in $\mathscr{L}_{-1}^2$ and also $\alpha_2\beta_N$ in $\mathscr{L}_{-1}^3$ give rise to different contributions to the spin correlation functions, which cancel to give 0.

APPENDIX G

In this appendix, we prove eq. (7.4). First we note that because of (2.22)

$$P_{j-1}^2 = 1, \quad \text{(G.1)}$$

so that

$$P_{j-1}\mathscr{H}_\sigma P_{j-1} = \mathscr{H}_\sigma - 4\alpha_{j-1}\beta_{j-1}[\mathscr{H}_\sigma, \alpha_{j-1}\beta_{j-1}]. \quad \text{(G.2)}$$

Using the commutation relations (4.18), (4.19) and again eq. (2.22) it follows that

$$\begin{aligned} P_{j-1}\mathscr{H}_\sigma P_{j-1} &= \mathscr{H}_\sigma + 4\mathrm{i}\alpha_{j-1}\beta_{j-1} \\ &\quad \times \Big(\sum_{k\neq j-1} (\mathsf{S}_\sigma)_{j-1\,k}\,\beta_k\beta_{j-1} - \sum_{k\neq j-1} (\mathsf{S}_\sigma)_{k\,j-1}\,\alpha_{j-1}\alpha_k\Big) \\ &= \mathscr{H}_\sigma - 2\mathrm{i}(S_1\alpha_{j-1}\beta_j + S_{-1}\alpha_j\beta_{j-1}) \\ &\quad - 2\mathrm{i}(S_1\alpha_{j-2}\beta_{j-1} + S_{-1}\alpha_{j-1}\beta_{j-2}). \end{aligned} \quad \text{(G.3)}$$

From eq. (G.3) with $j-1$ instead of j, and (2.22), we have

$$\begin{aligned} P_{j-2}P_{j-1}\mathscr{H}_\sigma P_{j-1}P_{j-2} &= \mathscr{H}_\sigma - 2\mathrm{i}(S_1\alpha_{j-2}\beta_{j-1} + S_{-1}\alpha_{j-1}\beta_{j-2}) \\ &\quad - 2\mathrm{i}(S_1\alpha_{j-3}\beta_{j-2} + S_{-1}\alpha_{j-2}\beta_{j-3}) \\ &\quad + 8\mathrm{i}\alpha_{j-2}\beta_{j-2}[S_1\alpha_{j-1}\beta_j + S_{-1}\alpha_j\beta_{j-1} \\ &\quad + S_1\alpha_{j-2}\beta_{j-1} + S_{-1}\alpha_{j-1}\beta_{j-2}]\,\alpha_{j-2}\beta_{j-2} \\ &= \mathscr{H}_\sigma - 2\mathrm{i}(S_1\alpha_{j-1}\beta_j + S_{-1}\alpha_j\beta_{j-1}) \\ &\quad - 2\mathrm{i}(S_1\alpha_{j-3}\beta_{j-2} + S_{-1}\alpha_{j-2}\beta_{j-3}). \end{aligned} \quad \text{(G.4)}$$

Proceeding in the same way, we find

$$P_2 \cdots P_{j-2}P_{j-1}\mathscr{H}_\sigma P_{j-1}P_{j-2} \cdots P_2$$

$$= \mathscr{H}_\sigma - 2\mathrm{i}\,(S_1\alpha_{j-1}\beta_j + S_{-1}\alpha_j\beta_{j-1}) - 2\mathrm{i}\,(S_1\alpha_1\beta_2 + S_{-1}\alpha_2\beta_1). \tag{G.5}$$

Applying eq. (G.2) for $j = 1$ and the commutation relations (4.28) and (4.29), we have

$$P_1\mathscr{H}_\sigma P_1 = \mathscr{H}_\sigma + 4\mathrm{i}\alpha_1\beta_1 \left(\sum_{k \neq 1} (\mathsf{S}_\sigma)_{1k}\,\beta_k\beta_1 - \sum_{k \neq 1} (\mathsf{S}_\sigma)_{k1}\,\alpha_1\alpha_k\right)$$

$$= \mathscr{H}_\sigma - 2\mathrm{i}\,(S_1\alpha_1\beta_2 + S_{-1}\alpha_2\beta_1) - 2\mathrm{i}\,[(\mathsf{S}_\sigma)_{1N}\,\alpha_1\beta_N + (\mathsf{S}_\sigma)_{N1}\,\alpha_N\beta_1]$$

$$= \mathscr{H}_\sigma - 2\mathrm{i}\,(S_1\alpha_1\beta_2 + S_{-1}\alpha_2\beta_1) - \sigma h, \tag{G.6}$$

where

$$h = -2\mathrm{i}\,(S_{-1}\alpha_1\beta_N + S_1\alpha_N\beta_1). \tag{G.7}$$

From (G.5), (G.6) and (2.22), it follows that

$$P_1 \cdots P_{j-1}\mathscr{H}_\sigma P_{j-1} \cdots P_1 = \mathscr{H}_\sigma - \sigma h - 2\mathrm{i}\,(S_1\alpha_{j-1}\beta_j + S_{-1}\alpha_j\beta_{j-1}). \tag{G.8}$$

Eq. (7.4) is obvious from (G.8) after multiplying both sides by $P_1 \cdots P_{j-1}$ using eq. (G.1).

APPENDIX H

In this appendix we prove the decoupling (7.19) for sufficiently large values of j. In the proof we shall restrict ourselves to the case that $j < \frac{1}{2}N$, $j + p < N$. (Similar considerations can be given for the case that $j > \frac{1}{2}N$, $j + p \leq N$. Then the decoupling is correct if $N - j$ is sufficiently large.) In order to evaluate the right-hand side of (7.14), we use the expansions

$$\alpha_j(\tau, \sigma) = \sum_{k_1=0}^{\infty} \frac{\tau^{k_1}}{k_1!} A_{k_1}, \tag{H.1}$$

$$\exp(\mathscr{L}_\sigma\tau) = \sum_{k_2=0}^{\infty} \frac{\tau^{k_2}}{k_2!} \mathscr{L}_\sigma^{k_2} \tag{H.2}$$

and

$$\exp(\mathscr{L}_{-\sigma,j}\tau)\left(\prod_{k=j}^{j+p-1} \frac{2}{\mathrm{i}}\,\alpha_k\beta_k\right)\alpha_{j+p} = \sum_{k_3=0}^{\infty} \frac{\tau^{k_3}}{k_3!} A_{k_3}. \tag{H.3}$$

Consider now the contributions of (7.14) for fixed values of k_1, k_2, k_3. It can be written as a sum of averages of products of operators α and β. These averages can be expressed in terms of pfaffians.

Let us choose j so large that $j \geq k_1 + k_2 + k_3$. Should the decoupling (7.19) be incorrect, we would have nonvanishing contributions from averages

$$\langle \varrho_\sigma \alpha_l \beta_m \rangle \qquad \text{or} \qquad \langle \varrho_\sigma \beta_l \alpha_m \rangle, \tag{H.4}$$

where the operator with index l originates from the expansion (H.2) and the operator with index m originates from (H.1) or (H.3). Without loss of generality we can restrict our considerations to the case that l is an index of order $\mathcal{O}(1)$, *cf.* eq. (4.8).

The averages (H.4) have the order of magnitude β^{m-l}, or even a higher power of β. Consider now the contribution for fixed values of k_1, k_2, k_3. The highest index l which can occur in $\mathcal{L}_\sigma^{k_2}$ is equal to k_2. The lowest index m occurring in A_{k_1} or A_{k_3} is equal to $j - \max(k_1, k_3)$, which is at least $j - (k_1 + k_3)$, so that

$$m - l \geq j - (k_1 + k_2 + k_3). \tag{H.5}$$

The contribution to the spin correlation function would have the order of magnitude

$$\tau^{k_1+k_2+k_3}\beta^{m-l}. \tag{H.6}$$

On the other hand, the spin correlation function can be written as a power series in τ and μ, *i.e.*

$$\langle \varrho_\sigma S_j^x(\tau,\sigma)\, S_{j+p}^x \rangle = \sum_{\lambda,\mu} c_{j\lambda\mu}^{(p)} \tau^\mu \beta^\lambda \tag{H.7}$$

and in a high-temperature expansion we can restrict ourselves to values λ and μ satisfying

$$\lambda + \mu \leq \nu - 1, \tag{H.8}$$

for some value of ν, *cf.* eq. (4.12).

Hence, the contribution (H.6) is irrelevant, if

$$k_1 + k_2 + k_3 + m - l > \nu - 1 \tag{H.9}$$

and (H.9) is satisfied if

$$j > \nu - 1, \tag{H.10}$$

so that for each value of ν we can ensure that the decoupling (7.19) is correct by choosing j in such a way that (H.10) is satisfied.

8. Remarks

A. The thermodynamic Wick theorem

Let A_1, A_2, ..., A_{2n} be arbitrary linear combinations of fermion creation and annihilation operators η_k and $\eta_k^\dagger$. Let

$$\rho \equiv e^{-\beta\mathcal{H}} \langle e^{-\beta\mathcal{H}} \rangle \tag{8.1}$$

be the density operator, corresponding to a hamiltonian $\mathcal{H}$, which is diagonal in terms of the operators $\eta_k^\dagger$ and η_k, i.e.

$$\mathcal{H} = \sum_k \lambda_k \eta_k^\dagger \eta_k \quad . \tag{8.2}$$

Then the thermodynamic Wick theorem reads

$$\langle \rho A_1 A_2 \ldots A_{2n} \rangle = \mathrm{Pf}(A_1, A_2, \ldots, A_{2n}) \ , \tag{8.3}$$

cf. eqs. (3.15) and (3.16) .

Eq. (8.3) can be proved by induction. For n = 1 eq. (8.3) is trivial, so we may assume that the Wick theorem is valid for products consisting of 2n-2 operators A. Furthermore A_1 may be chosen to be equal to one of the creation or annihilation operators $\eta_k^\dagger$ or η_k resp., since the extension to operators A_1 which are linear combinations is trivial. In the proof use is made of the KMS-property

$$\langle \rho A_2 \ldots A_{2n} A_1 \rangle = \langle \rho A_1(\beta) A_2 \ldots A_{2n} \rangle \quad , \tag{8.4}$$

where

$$A_1(\beta) \equiv e^{\beta\mathcal{H}} A_1 e^{-\beta\mathcal{H}} . \tag{8.5}$$

From (8.2) one has

$$\frac{dA_1(\beta)}{d\beta} = [\mathcal{H}, A_1(\beta)] = \pm \lambda_k A_1(\beta) \quad , \tag{8.6}$$

where the + and - signs refer to the two cases that $A_1 = \eta_k^\dagger$ and $A_1 = \eta_k$ resp. From (8.4) and (8.6), it follows that

$$\langle \rho A_2 \ldots A_{2n} A_1 \rangle = e^{\pm\beta\lambda_k} \langle \rho A_1 A_2 \ldots A_{2n} \rangle \ , \tag{8.7}$$

or equivalently

$$\langle \rho A_1 A_2 \ldots A_{2n} \rangle + \langle \rho A_2 \ldots A_{2n} A_1 \rangle = g_k^{-1} \langle \rho A_1 A_2 \ldots A_{2n} \rangle \quad , \tag{8.8}$$

where g_k can be expressed in terms of the Fermi-Dirac distribution f_k:

$$g_k = \begin{cases} (e^{\beta\lambda_k} + 1)^{-1} = f_k \quad , \text{ if } A_1 = \eta_k^\dagger \\ (e^{-\beta\lambda_k} + 1)^{-1} = 1 - f_k \ , \text{ if } A_1 = \eta_k \ . \end{cases} \tag{8.9}$$

For the anticommutator of A_1 and an operator A_j, which is a linear combination of the operators η and $\eta^\dagger$, we have the relation

$$g_k\{A_1, A_j\} = \langle \rho A_1 A_j \rangle \ . \tag{8.10}$$

Eq. (8.10) is obvious noting that A_j can be written as $A_j = cA_1^\dagger$ + other terms, so that the left-and right-hand side of (8.10) are equal to cg_k, in view of the anticommutation relations and the connection between g_k and the Fermi-Dirac distribution.

Using eq. (8.8), the anticommutation relations and eq. (8.10), we have

$$\begin{aligned} \langle \rho A_1 A_2 \ldots A_{2n} \rangle &= g_k\{ \langle \rho A_1 A_2 \ldots A_{2n} \rangle + \langle \rho A_2 \ldots A_{2n} A_1 \rangle \} = \\ &= g_k \sum_{j=2}^{2n} (-1)^{j-2} \{A_1, A_j\} \langle \rho A_2 A_3 \ldots \cancel{A_j} \ldots A_{2n} \rangle = \\ &= \sum_{j=2}^{2n} (-1)^{j-2} \langle \rho A_1 A_j \rangle \langle \rho A_2 A_3 \ldots \cancel{A_j} \ldots A_{2n} \rangle \ , \end{aligned} \tag{8.11}$$

where $A_2 A_3 \ldots \cancel{A_j} \ldots A_{2n}$ is a shorthand notation for $A_2 A_3 \ldots A_{j-1} A_{j+1} \ldots A_{2n}$, i.e. the operator A_j has been omitted in the product of operators $A_2 \ldots A_{2n}$. Using the induction hypothesis, we have

$$\langle \rho A_1 A_2 \ldots A_{2n} \rangle = \sum_{j=2}^{2n} (-1)^{j-2} \langle \rho A_1 A_j \rangle \mathrm{Pf}(A_2, A_3, \ldots, \cancel{A_j}, \ldots, A_{2n}) \ . \tag{8.12}$$

Eq. (8.3) is obvious from (8.12) because of the recursion relation, by which a pfaffian involving 2n operators can be expressed as a linear combination of pfaffians with 2n-2 operators.

In this remark we proved the thermodynamic Wick theorem for fermion operators. In the case of boson operators one can give a similar formulation in terms of so-called hafnians [11)], which are similar to the right-hand side of eq. (3.15) apart from the absence of the factor $(-1)^{\nu(P)}$. The proof proceeds along the same lines, using the commutation relations and the Bose-Einstein distribution.

B. Note on the difference between the a-cyclic and c-cyclic version of the XY model

In section 7 we have shown on the basis of a high-temperature expansion that

$$\chi_c \neq \chi_a, \tag{8.13}$$

for the xx element of the susceptibility tensor per particle in the thermodynamic limit, as defined by eq. (3.1) and (3.2) for $\mathcal{H} = \mathcal{H}_c$ and $\mathcal{H} = \mathcal{H}_a$ resp., where $\mathcal{H}_c$ and $\mathcal{H}_a$ are the hamiltonians for the c-cyclic and a-cyclic version of the XY model, cf. eqs. (2.7) and (2.1) resp.

Eq. (8.13) is a direct consequence of the factorization property (7.20), which can be written

$$\langle \rho_c e^{\tau\mathcal{H}_c} S_j^x e^{-\tau\mathcal{H}_c} S_{j+p}^x \rangle =$$

$$= \langle \rho_a e^{\tau\mathcal{H}_a} S_j^x e^{-\tau\mathcal{H}_a} S_{j+p}^x \rangle \langle \rho_c e^{\tau\mathcal{H}_c} e^{-\tau(\mathcal{H}_c+h)} \rangle , \tag{8.14}$$

where ρ_c and ρ_a are the density operators associated with $\mathcal{H}_c$ and $\mathcal{H}_a$. Eq. (8.14) is valid up to an arbitrary order in β, for sufficiently large values of j and N-j-p.

If one defines susceptibilities $\tilde{\chi}_c$ and $\tilde{\chi}_a$ by interchanging the two limits $N \to \infty$, $B_x \to 0$ in eq. (3.1), then both susceptibilities should be equal. This follows from the relation

$$f[\mathcal{H}_c - B_x M_x] = f[\mathcal{H}_a - B_x M_x] \tag{8.15}$$

for the free energy per particle in the thermodynamic limit, since the difference between the hamiltonians occurring at the left- and right-hand side is only a boundary term. Since there is no reason to doubt the validity of the relation $\chi_a = \tilde{\chi}_a$, it follows that $\chi_c \neq \tilde{\chi}_c$, i.e. in the calculation of χ_c the two limiting procedures $N \to \infty$, $B_x \to 0$ and $B_x \to 0$, $N \to \infty$ cannot be interchanged.

A more explicit illustration of (8.13) can be given by considering the simple case of the Ising model 16) in the absence of a magnetic field, i.e. $\gamma = 1$, $B = 0$. The a-cyclic and c-cyclic hamiltonian are given by

$$\mathcal{H}_a = 2 \sum_{j=1}^{N} S_j^x S_{j+1}^x , \quad \mathcal{H}_c = \mathcal{H}_a - 2S_1^x S_N^x (1+P), \tag{8.16}$$

cf. e.g. (2.1)-(2.4), (2.6), (2.8) and (2.9). Using the (anti)commutation relations (2.35) and (2.36), the autocorrelation function of the magnetization per particle can be written

$$R_c(\tau) \equiv \lim_{N\to\infty} N^{-1}\Big[\langle \rho_c e^{\tau\mathcal{H}_c} M_x e^{-\tau\mathcal{H}_c} M_x\rangle - \langle \rho_c M_x\rangle^2\Big]$$

$$= \lim_{N\to\infty} N^{-1}\langle \rho_c e^{\tau(\mathcal{H}_a - 2S_1^xS_N^x)(1+P)} M_x^2\, e^{-\tau(\mathcal{H}_a - 2S_1^xS_N^x)(1-P)}\rangle$$

$$= \lim_{N\to\infty} N^{-1}\langle \rho_c e^{-4\tau S_1^xS_N^xP} M_x^2\rangle \quad . \tag{8.17}$$

Using the α and β operators, defined by eq. (2.21), the Wick theorem (3.15) and eqs. (3.17)-(3.19) for the averages, the autocorrelation function per particle can be evaluated to be

$$R_c(\tau) = (\cosh\tau - \sinh\tau\tanh\tfrac{1}{2}\beta)R_a \ , \tag{8.18}$$

where $R_a = \frac{1}{4}e^{-\beta}$ is the autocorrelation function in the a-cyclic model. Integrating (8.18) it is found that

$$\chi_c = \int_0^\beta d\tau\, R_c(\tau) = \tfrac{1}{2}e^{-\beta}\tanh\tfrac{1}{2}\beta \neq \chi_a = \tfrac{1}{4}\beta e^{-\beta} \quad . \tag{8.19}$$

The time-dependent autocorrelation function in the c-cyclic model can be found substituting $\tau = it$ and

$$R_c(it) = \tfrac{1}{4}e^{-\beta}(\cos t + i\sin t\tanh\tfrac{1}{2}\beta) \quad . \tag{8.20}$$

In the c-cyclic model, $R_c(it)$ is no longer a constant, but time-dependent, in contrast with the (normal) a-cyclic Ising model, where there is no time-dependence. This illustrates the difficulties which can arise if the c-cyclic model is used in the evaluation of physical quantities. For more details see ref. 16.

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II. ON THE ANISOTROPIC HEISENBERG CHAIN

1. Introduction

In this paper we consider a linear chain of N spins $\frac{1}{2}$ with nearest-neighbour interactions. These interactions are assumed to be completely anisotropic, *i.e.*, the coupling constants between the x, y and z components are denoted by J_1, J_2, J_3 respectively and are chosen to be different. Recently, this model has received a great deal of interest, in view of the exact result for the ground state obtained by Baxter^1).

In the present paper we investigate the high-temperature expansion for the specific heat c per spin and the zz component χ_{zz} of the susceptibility tensor per spin in the absence of a magnetic field ($B = 0$). For the isotropic case ($J_1 = J_2 = J_3 = J$) high-temperature expansions containing many powers of the inverse temperature $\beta = (kT)^{-1}$ can be found in a paper by Baker, Rushbrooke and Gilbert^2). The case of axial symmetry $J_1 = J_2 \neq J_3$ has been investigated by Wood and Dalton^3) up to the order β^7 for arbitrary spins and arbitrary lattices.

For an anisotropic chain with spins $\frac{1}{2}$ use can be made of a perturbation calculation, in which the zz coupling between the spins characterized by J_3 is assumed to be a small perturbation as compared to the other interactions which form the hamiltonian of the so-called XY model. This model, which is exactly soluble, has been investigated by many authors$^{4-8}$).

The idea of applying a perturbation calculation to the anisotropic Heisenberg chain has been discussed before by Katsura and Inawashiro9). As a result of such a calculation the logarithm of the partition function per particle $\ln z$ can be expressed in terms of integrals $\int_0^{2\pi} \mathrm{d}\phi \, f(\phi, \beta)$, which in general require a numerical evaluation.

The perturbational approach may be especially useful in the derivation of a high-temperature expansion. After expanding the integrand $f(\phi, \beta)$ in powers of β, the coefficients turn out to be simple polynomials in $\cos\phi$ and $\sin\phi$ and the remaining integration is trivial.

In the present paper we shall restrict our investigations to a first-order perturbation calculation. Using the first-order results in the coupling constant J_3, the exact results of the *XY* model and the high-temperature expansion for the isotropic one-dimensional Heisenberg chain derived by Baker *et al.*2), we can determine all the coefficients of the expansion of the logarithm of the partition function per particle $\ln z$ in the absence of a magnetic field up to the order β^9. As a corollary we obtain the high-temperature expansion of the difference $\ln z^{\mathrm{af}} - \ln z^{\mathrm{f}}$ between the logarithm of the partition function per particle in the antiferromagnetic case and the corresponding quantity in the ferromagnetic case up to the order β^{12}.

Using similar considerations we obtain the high-temperature expansion of the susceptibility χ_{zz} in the absence of a magnetic field up to order β^6. In the derivation use is made of a high-temperature expansion for the so-called transverse susceptibility χ_{xx} in the anisotropic *XY* model (with $J_3 = 0$). This quantity has been investigated in detail in a previous paper10), where we have also shown that the so-called c-cyclic version of the *XY* model gives rise to an incorrect result, even in the thermodynamic limit.

One of the reasons for restricting ourselves to a first-order calculation is to demonstrate explicitly the simple way in which one can derive the coefficients of reasonable powers in the high-temperature expansion. Second- and higher-order perturbation calculation will be more laborious, but certainly not impossible, and this can lead eventually to some additional coefficients in the high-temperature expansions. By using a Padé-approximant analysis in the same way as Baker *et al.*2) for the isotropic case one can obtain results which are reliable at relatively low temperatures.

On the other hand, numerical calculations on finite chains of spins can give quite accurate information on physical quantities in the thermodynamic limit. For the case of axial symmetry and spin $S=\frac{1}{2}$ such calculations have been done by Bonner and Fisher 11). Very recently Blöte12) has extended these calculations taking into account higher spin values $S \geq 1$ and the effect of crystalline fields. As far as we know no finite-chain calculations have been performed for the completely anisotropic case. Apart from this, a high-temperature expansion with exact expressions for the coefficients can be of interest in itself.

The paper is arranged as follows. In section 2 we review some of the relevant properties of the XY model and the first-order calculation in J_3 is performed in detail. The high-temperature expansion for $\ln z$ in the absence of a magnetic field is derived in section 3 and in section 4 we give the high-temperature expansion for the susceptibility χ_{zz}.

Finally, in section 5 we present some figures containing curves of c and χ_{zz} *vs.* β for various values of the interaction parameters. These figures show some characteristic features of deviations from axial symmetry in the high-temperature region. In general, the consequences of such deviations seem to be more important in the case of ferromagnetic interactions. For the χ_{zz} susceptibility the effects are very small, if the axis of axial symmetry coincides with the z direction. However, if this axis is perpendicular to the z direction, the dependence on the deviations is much larger. This corroborates the conclusions obtained in a previous paper on the XY model[10]). There it was shown that the transverse susceptibility χ_{xx} shows a large dependence on the anisotropy parameter γ, in contrast with the very weak dependence of the susceptibility χ_{zz}.

2. First-order perturbation calculation

In this section we consider the zz interaction as a perturbation. The hamiltonian can be written

$$\mathscr{H} = \mathscr{H}_{XY} + \mathscr{H}_1, \tag{2.1}$$

where

$$\mathscr{H}_{XY} = J_1 \sum_{j=1}^{N} S_j^x S_{j+1}^x + J_2 \sum_{j=1}^{N} S_j^y S_{j+1}^y - B \sum_{j=1}^{N} S_j^z \tag{2.2}$$

and

$$\mathscr{H}_1 = J_3 \sum_{j=1}^{N} S_j^z S_{j+1}^z, \qquad (S_{N+1} \equiv S_1). \tag{2.3}$$

Using a Dyson series expansion, the logarithm of the partition function can be written

$$\ln Z = \ln Z_{XY} - \int_0^\beta \mathrm{d}\tau \, \langle \varrho_{XY} \mathscr{H}_1(\tau) \rangle + \frac{1}{2} \int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \, \langle \varrho_{XY} [\mathscr{H}_1(\tau_1) - \langle \varrho_{XY} \mathscr{H}_1 \rangle] [\mathscr{H}_1(\tau_2) - \langle \varrho_{XY} \mathscr{H}_1 \rangle] \rangle + \cdots, \tag{2.4}$$

where Z and Z_{XY} are the partition functions corresponding to the hamiltonian $\mathscr{H}$ as given by eq. (2.1) and the hamiltonian $\mathscr{H}_{XY}$ of the XY model, respectively, and where ϱ_{XY} is the density operator of the XY model, *i.e.*,

$$Z \equiv \operatorname{Tr} e^{-\beta\mathscr{H}}, \qquad Z_{XY} \equiv \operatorname{Tr} e^{-\beta\mathscr{H}_{XY}}, \qquad \varrho_{XY} \equiv Z_{XY}^{-1}\, e^{-\beta\mathscr{H}_{XY}}, \tag{2.5}$$

and where $A(\tau)$ for an arbitrary operator A is defined by

$$A(\tau) \equiv e^{\tau\mathscr{H}_{XY}} A\, e^{-\tau\mathscr{H}_{XY}}. \tag{2.6}$$

In a first-order perturbation calculation, eq. (2.4) reduces to

$$\ln Z = \ln Z_{XY} - \beta J_3 \sum_{j=1}^{N} \langle \varrho_{XY} S_j^z S_{j+1}^z \rangle. \tag{2.7}$$

In the thermodynamic limit $N \to \infty$, both quantities per spin, *i.e.*, $N^{-1} \ln Z_{XY}$ and the nearest-neighbour spin correlation function can be calculated by using the so-called c-cyclic version of the XY hamiltonian. Using the same considerations as in refs. 7 and 8, the hamiltonian of the c-cyclic XY model can be written

$$\mathscr{H}_{-1} = \mathrm{i} \sum_{j,k=1}^{N} \alpha_j S_{jk} \beta_k, \tag{2.8}$$

where the operators α_j and β_j are defined by using the Jordan–Wigner transformation

$$\begin{aligned} \alpha_1 &= S_1^x \sqrt{2}, \qquad \alpha_j = \left(\prod_{k=1}^{j-1} -2S_k^z\right) S_j^x \sqrt{2}, \\ \beta_1 &= -S_1^y \sqrt{2}, \qquad \beta_j = -\left(\prod_{k=1}^{j-1} -2S_k^z\right) S_j^y \sqrt{2} \qquad (j = 2, \ldots, N). \end{aligned} \tag{2.9}$$

They satisfy the anticommutation rules

$$\{\alpha_i, \alpha_j\} = \delta_{ij}, \qquad \{\beta_i, \beta_j\} = \delta_{ij}, \qquad \{\alpha_i, \beta_j\} = 0. \tag{2.10}$$

In eq. (2.8) the cyclic matrix S is defined by

$$\begin{aligned} S_{jk} &= S_{k-j}, \\ S_n &= \tfrac{1}{2} J_1 (\delta_{n,-1} + \delta_{n,N-1}) + \tfrac{1}{2} J_2 (\delta_{n,1} + \delta_{n,1-N}) - B\delta_{n,0} \\ &\qquad (n = 1 - N, \ldots, N - 1). \end{aligned} \tag{2.11}$$

In the thermodynamic limit, by using the same lines of reasoning as in refs. 7 and 8, it can be shown that

$$\ln z_{XY} \equiv \lim_{N\to\infty} N^{-1} \ln Z_{XY} = \lim_{N\to\infty} N^{-1} \ln Z_{-1}, \tag{2.12}$$

$$\lim_{N\to\infty} \langle \varrho_{XY} S_j^z S_{j+1}^z \rangle = - \lim_{N\to\infty} \langle \varrho_{-1} \alpha_j \beta_j \alpha_{j+1} \beta_{j+1} \rangle. \tag{2.13}$$

Here Z_{-1} and ϱ_{-1} are the partition function and the density operator of the c-cyclic XY model, *i.e.*,

$$Z_{-1} \equiv \mathrm{Tr}\, \mathrm{e}^{-\beta \mathscr{H}_{-1}}, \qquad \varrho_{-1} \equiv Z_{-1}^{-1}\, \mathrm{e}^{-\beta \mathscr{H}_{-1}}. \tag{2.14}$$

We have

$$\ln Z_{-1} = N \ln 2 + \sum_{k=1}^{N} \ln\left(\cosh \tfrac{1}{2}\beta \Lambda_k\right), \tag{2.15}$$

where Λ_k^2 $(k = 1, \ldots, N)$ are the eigenvalues of the symmetric cyclic matrix

$$\mathsf{M} \equiv \mathsf{S}\tilde{\mathsf{S}} = \tilde{\mathsf{S}}\mathsf{S}, \tag{2.16}$$

i.e.,

$$\Lambda_k^2 = [\tfrac{1}{2}(J_1 + J_2)\cos\varphi_k - B]^2 + [\tfrac{1}{2}(J_1 - J_2)\sin\varphi_k]^2, \qquad \varphi_k = k(2\pi/N). \tag{2.17}$$

In the thermodynamic limit we have from (2.12), (2.15) and (2.17)

$$\ln z_{XY} = \ln 2 + (1/2\pi)\int_0^{2\pi} \mathrm{d}\varphi \times \ln\left(\cosh \tfrac{1}{2}\beta\, \{[\tfrac{1}{2}(J_1 + J_2)\cos\varphi - B]^2 + [\tfrac{1}{2}(J_1 - J_2)\sin\varphi]^2\}^{\frac{1}{2}}\right). \tag{2.18}$$

The right-hand side of eq. (2.13) can be evaluated by using the thermodynamic Wick theorem^{13}) and the expressions (*cf.* ref. 7)

$$\langle \varrho_{-1}\alpha_j\alpha_k\rangle = \langle \varrho_{-1}\beta_j\beta_k\rangle = \tfrac{1}{2}\delta_{jk}, \tag{2.19}$$

$$\langle \varrho_{-1}\alpha_j\beta_k\rangle = \tfrac{1}{2}\mathrm{i}\,(\mathsf{S}\mathsf{M}^{-\frac{1}{2}} \tanh \tfrac{1}{2}\beta \mathsf{M}^{\frac{1}{2}})_{k-j}. \tag{2.20}$$

In first-order perturbation calculation (*i.e.* first order in the coupling constant J_3 corresponding to the zz interaction) the logarithm of the partition function per spin can be written

$$\ln z \equiv \lim_{N\to\infty} N^{-1} \ln Z = \ln z_{XY} - \beta J_3 \lim_{N\to\infty} \langle \varrho_{-1} S_j^z S_{j+1}^z\rangle, \tag{2.21}$$

where $\ln z_{XY}$ has been given by (2.18) and where

$$-\beta J_3 \langle \varrho_{-1} S_j^z S_{j+1}^z\rangle = \tfrac{1}{4}\beta J_3 \left[(\mathsf{S}\mathsf{M}^{-\frac{1}{2}} \tanh \tfrac{1}{2}\beta \mathsf{M}^{\frac{1}{2}})_1 (\mathsf{S}\mathsf{M}^{-\frac{1}{2}} \tanh \tfrac{1}{2}\beta \mathsf{M}^{\frac{1}{2}})_{-1} - (\mathsf{S}\mathsf{M}^{-\frac{1}{2}} \tanh \tfrac{1}{2}\beta \mathsf{M}^{\frac{1}{2}})_0^2\right]. \tag{2.22}$$

3. High-temperature expansion for $\ln z$

In this section we derive the high-temperature expansion up to order β^9 for $\ln z$ of the anisotropic one-dimensional Heisenberg model with spin $S = \frac{1}{2}$ (J_1, J_2, J_3 being different).

The high-temperature expansion in the absence of a magnetic field ($B = 0$) can be written

$$\ln z = \sum_{\nu_1, \nu_2, \nu_3} c_{\nu_1\nu_2\nu_3} \beta^{\nu_1+\nu_2+\nu_3} J_1^{\nu_1} J_2^{\nu_2} J_3^{\nu_3}. \tag{3.1}$$

Here

$$c_{\nu_1\nu_2\nu_3} = 0 \quad \begin{cases} \text{unless} & \nu_1, \nu_2, \nu_3 \quad \text{are even,} \\ \text{or} & \nu_1, \nu_2, \nu_3 \quad \text{are odd.} \end{cases} \tag{3.2}$$

This can be seen as follows. By expanding the exponential $\exp(-\beta\mathscr{H})$ the partition function can be expressed in terms of sums of products

$$\prod_k \operatorname{tr}_k f_k(S_k^x, S_k^y, S_k^z), \tag{3.3}$$

where tr_k is the trace over the two-dimensional space of spin k and $f_k(S_k^x, S_k^y, S_k^z)$ can be expressed as a sum of terms each of which contains the components of spin k in an arbitrary order. Only those terms which contain each of the operators S_k^x, S_k^y, S_k^z an even number of times or each of them an odd number of times can give a nonvanishing contribution to tr_k. From this eq. (3.2) is obvious.

Furthermore the coefficients $c_{\nu_1\nu_2\nu_3}$ are invariant under permutations of ν_1, ν_2, ν_3, *i.e.*,

$$c_{\nu_1\nu_2\nu_3} = c_{\nu_{P1}\nu_{P2}\nu_{P3}}, \tag{3.4}$$

where $(P1, P2, P3)$ is an arbitrary permutation of (1, 2, 3). Using (3.1), (3.2) and (3.4) the expansion of $\ln z$ up to order β^9 can be written

$$\begin{aligned} \ln z = {} & \ln 2 + (\beta/4)^2 \tfrac{1}{2} [a_{200} (J_1^2 + \text{cycl.})] + (\beta/4)^3 a_{111} J_1 J_2 J_3 \\ & - (\beta/4)^4 \tfrac{1}{12} [a_{400} (J_1^4 + \text{cycl.}) + a_{220} (J_1^2 J_2^2 + \text{cycl.})] \\ & - (\beta/4)^5 [a_{311} (J_1^3 J_2 J_3 + \text{cycl.})] + (\beta/4)^6 \tfrac{1}{90} \{a_{600} (J_1^6 + \text{cycl.}) \\ & + a_{420} [(J_1^4 J_2^2 + J_1^2 J_2^4) + \text{cycl.}] + a_{222} J_1^2 J_2^2 J_3^2\} \\ & + (\beta/4)^7 \tfrac{1}{45} [a_{511} (J_1^5 J_2 J_3 + \text{cycl.}) + a_{331} (J_1^3 J_2^3 J_3 + \text{cycl.})] \\ & - (\beta/4)^8 \tfrac{1}{2520} \{a_{800} (J_1^8 + \text{cycl.}) + a_{620} [(J_1^6 J_2^2 + J_1^2 J_2^6) + \text{cycl.}] \end{aligned}$$

$$
\begin{aligned}
&+ a_{440}(J_1^4J_2^4 + \text{cycl.}) + a_{422}(J_1^4J_2^2J_3^2 + \text{cycl.})\} \\
&- (\beta/4)^9 \tfrac{1}{189} \{a_{711}(J_1^7J_2J_3 + \text{cycl.}) \\
&+ a_{531}[(J_1^5J_2^3J_3 + J_1^3J_2^5J_3) + \text{cycl.}] + a_{333}J_1^3J_2^3J_3^3\},
\end{aligned}
\tag{3.5}
$$

where $f(J_1\ J_2, J_3)$ + cycl. denotes $f(J_1, J_2, J_3) + f(J_3, J_1, J_2) + f(J_2, J_3, J_1)$. The numerical factors appearing in (3.5) are introduced for reasons of convenience. (All coefficients $a_{\nu_1\nu_2\nu_3}$ will turn out to be integers.)

The coefficients $a_{\nu_1\nu_2\nu_3}$ with $\nu_3 = 0$ can be obtained from a high-temperature expansion of $\ln z_{XY}$. By expanding the ln (cosh ...) in eq. (2.18) and by carrying out the trivial integrations over ϕ, we obtain the result

$$
\begin{aligned}
\ln z_{XY} = \ln 2 &+ (\beta/4)^2 \tfrac{1}{2}(J_1^2 + J_2^2) \\
&- (\beta/4)^4 \tfrac{1}{12}(J_1^4 + J_2^4 + 4J_1^2J_2^2) \\
&+ (\beta/4)^6 \tfrac{1}{45}(J_1^6 + J_2^6 + 9J_1^4J_2^2 + 9J_1^2J_2^4) \\
&- (\beta/4)^8 \tfrac{1}{2520}[17(J_1^8 + J_2^8) + 272(J_1^6J_2^2 + J_1^2J_2^6) + 612J_1^4J_2^4].
\end{aligned}
\tag{3.6}
$$

Hence

$$
\begin{aligned}
&a_{200} = 1, \quad a_{400} = 1, \quad a_{220} = 4, \quad a_{600} = 2, \\
&a_{420} = 18, \quad a_{800} = 17, \quad a_{620} = 272, \quad a_{440} = 612.
\end{aligned}
\tag{3.7}
$$

The coefficients $a_{\nu_1\nu_2 1}$, *i.e.* in particular the coefficients a_{111}, a_{311}, a_{511}, a_{331}, a_{711}, a_{531}, can be obtained by applying the first-order perturbation calculation given in section 2, *cf.* eq. (2.22). By using a high-temperature expansion for the matrix-elements $(\mathrm{S}\mathrm{M}^{-\frac{1}{2}} \tanh \tfrac{1}{2}\beta \mathrm{M}^{\frac{1}{2}})_n$, $(n = -1, 0, 1)$, it is found that

$$
\begin{aligned}
&-\beta J_3 \langle \varrho_{-1} S_j^z S_{j+1}^z \rangle \\
&\quad = (\beta/4)^3 J_1J_2J_3 - (\beta/4)^5 J_3(J_1^3J_2 + J_1J_2^3) \\
&\qquad + (\beta/4)^7 (J_3/45)[34(J_1^5J_2 + J_1J_2^5) + 97J_1^3J_2^3] \\
&\qquad - (\beta/4)^9 (J_3/189)[93(J_1^7J_2 + J_1J_2^7) + 516(J_1^5J_2^3 + J_1^3J_2^5)] \\
&\qquad + (\beta/4)^{11} (J_3/4725)[1382(J_1^9J_2 + J_1J_2^9) + 12551(J_1^7J_2^3 + J_1^3J_2^7) \\
&\qquad + 24424J_1^5J_2^5].
\end{aligned}
\tag{3.8}
$$

Hence

$$
\begin{aligned}
&a_{111} = 1, \quad a_{311} = 1, \quad a_{511} = 34, \quad a_{331} = 97, \\
&a_{711} = 93, \quad a_{531} = 516.
\end{aligned}
\tag{3.9}
$$

So far we have obtained all coefficients in (3.5) apart from a_{222}, a_{422} and a_{333}, occurring in the terms proportional to β^6, β^8 and β^9, respectively. These coefficients can be determined by using the high-temperature expansion for the isotropic Heisenberg chain, derived by Baker *et al.*[2]). The expansion is given by

$$\begin{aligned}\ln z = \ln 2 &+ \tfrac{3}{2}(\beta J/4)^2 + (\beta J/4)^3 - \tfrac{5}{4}(\beta J/4)^4 \\ &- 3(\beta J/4)^5 + \tfrac{7}{10}(\beta J/4)^6 + \tfrac{131}{15}(\beta J/4)^7 + \tfrac{1417}{280}(\beta J/4)^8 \\ &- \tfrac{4303}{189}(\beta J/4)^9 - \tfrac{334433}{9450}(\beta J/4)^{10} + \tfrac{23891}{525}(\beta J/4)^{11} + \cdots .\end{aligned} \tag{3.10}$$

This expansion follows from eq. (3.5) in ref. 2 by substituting $K = -\tfrac{1}{4}\beta J$, $\bar{H} = 0$.

Now the remaining coefficients can be found from eq. (3.5) by inserting $J_1 = J_2 = J_3 = J$. We have the equations

$$\begin{aligned}&3a_{600} + 6a_{420} + a_{222} = 63, \\ &a_{800} + 2a_{620} + a_{440} + a_{422} = -4251, \\ &3a_{711} + 6a_{531} + a_{333} = 4303.\end{aligned} \tag{3.11}$$

Using (3.7) and (3.9) we have

$$a_{222} = -51, \qquad a_{422} = -5424, \qquad a_{333} = 928. \tag{3.12}$$

We now have determined all the coefficients up to order β^9. The result is

$$\begin{aligned}\ln z = \ln 2 &+ (\beta/4)^2\, \tfrac{1}{2}(J_1^2 + \text{cycl.}) + (\beta/4)^3 J_1 J_2 J_3 \\ &- (\beta/4)^4\, \tfrac{1}{12}[(J_1^4 + \text{cycl.} + 4(J_1^2 J_2^2 + \text{cycl.})] - (\beta/4)^5 (J_1^3 J_2 J_3 + \text{cycl.}) \\ &+ (\beta/4)^6\, \tfrac{1}{90}\{2(J_1^6 + \text{cycl.}) + 18[(J_1^4 J_2^2 + J_1^2 J_2^4) + \text{cycl.}] - 51 J_1^2 J_2^2 J_3^2\} \\ &+ (\beta/4)^7\, \tfrac{1}{45}[34(J_1^5 J_2 J_3 + \text{cycl.}) + 97(J_1^3 J_2^3 J_3 + \text{cycl.})] \\ &- (\beta/4)^8\, \tfrac{1}{2520}\{17(J_1^8 + \text{cycl.}) + 272[(J_1^6 J_2^2 + J_1^2 J_2^6) + \text{cycl.}] \\ &+ 612(J_1^4 J_2^4 + \text{cycl.}) - 5424(J_1^4 J_2^2 J_3^2 + \text{cycl.})\} \\ &- (\beta/4)^9\, \tfrac{1}{189}\{93(J_1^7 J_2 J_3 + \text{cycl.}) \\ &+ 516[(J_1^5 J_2^3 J_3 + J_1^3 J_2^5 J_3) + \text{cycl.}] + 928 J_1^3 J_2^3 J_3^3\}.\end{aligned} \tag{3.13}$$

3.1. *Remarks*

i) In contrast with the coefficients of order β^{10}, we can also calculate the coefficients of order β^{11} by a first-order perturbation calculation. There are four coefficients a_{911}, a_{731}, a_{551} and a_{533}. The first three of them are given by the expansion (3.8); the remaining coefficient a_{533} can be determined from (3.10). As a result we can write down the high-temperature expansion $\ln z^{\mathrm{af}} - \ln z^{\mathrm{f}}$ up to order β^{12}, where z^{af} refers to the antiferromagnetic case $J_1, J_2, J_3 > 0$ and z^{f} to the ferromagnetic case $J_1, J_2, J_3 < 0$. We have

$$\begin{aligned}
\tfrac{1}{2}(\ln z^{\mathrm{af}} - \ln z^{\mathrm{f}}) = & \sum_{\substack{\nu_1, \nu_2, \nu_3 = \text{odd} \\ \nu_1+\nu_2+\nu_3 \leqslant 9}} c_{\nu_1\nu_2\nu_3} \beta^{\nu_1+\nu_2+\nu_3} J_1^{\nu_1} J_2^{\nu_2} J_3^{\nu_3} \\
& + (\beta/4)^{11} \tfrac{1}{4725} \{1382\,(J_1^9 J_2 J_3 + \text{cycl.}) \\
& + 12551\,[(J_1^7 J_2^3 J_3 + J_1^3 J_2^7 J_3) + \text{cycl.}] \\
& + 24424\,(J_1^5 J_2^5 J_3 + \text{cycl.}) + 20765\,(J_1^5 J_2^3 J_3^3 + \text{cycl.})\} \\
& + \mathcal{O}(\beta^{13}),
\end{aligned} \tag{3.14}$$

where the coefficients $c_{\nu_1\nu_2\nu_3}$ with $\nu_1 + \nu_2 + \nu_3 \leq 9$ have been given in the right-hand side of (3.13).

ii) The coefficients corresponding to the order β^{10} cannot be determined in this way. There are five coefficients a_{1000}, a_{820}, a_{640}, a_{622}, a_{442}, three of which can be calculated from $\ln z_{XY}$. In order to distinguish the two remaining coefficients a_{622} and a_{442} one has to carry out a second-order perturbation calculation, which lies outside the scope of this paper. Using second-order perturbation and the Baker expansion one can also determine the coefficients of β^{12} and β^{14}. For the order β^{13}, however, a third-order perturbation calculation is needed.

4. High-temperature expansion for χ_{zz}

In this section we derive the high-temperature expansion for the susceptibility χ_{zz} up to order β^6 for the completely anisotropic Heisenberg chain, in the absence of a magnetic field ($B = 0$). This expansion can be written

$$\chi_{zz} = \sum_{\nu_1, \nu_2, \nu_3} d_{\nu_1\nu_2\nu_3} \beta^{\nu_1+\nu_2+\nu_3+1} J_1^{\nu_1} J_2^{\nu_2} J_3^{\nu_3}, \tag{4.1}$$

where

$$d_{\nu_1\nu_2\nu_3} = 0, \quad \begin{bmatrix} \text{unless} & \nu_1 & \text{and} & \nu_2 & \text{are even,} \\ \text{or} & \nu_1 & \text{and} & \nu_2 & \text{are odd.} \end{bmatrix} \tag{4.2}$$

This can be seen by expanding the partition function in a similar way as in eq. (3.3), but now the Zeeman term $-B\sum_l S_l^z$ should also be taken into account. Again, only the terms which contain each of the three components S_k^x, S_k^y, S_k^z an even number of times (or an odd number of times) can give a nonvanishing contribution to $\mathrm{tr}_k f_k(S_k^x, S_k^y, S_k^z)$. From this eq. (4.2) is obvious. The exponent $\nu_1 + \nu_2 + \nu_3 + 1$ of β follows from the thermodynamic relation

$$\chi_{zz} = \beta^{-1} \frac{\partial^2 \ln z}{\partial B^2}, \tag{4.3}$$

noting that for the calculation of the susceptibility in zero field we can restrict ourselves to quadratic terms in B.

Furthermore the χ_{zz} susceptibility is invariant for rotations around the z axis, *i.e.*

$$d_{\nu_1\nu_2\nu_3} = d_{\nu_2\nu_1\nu_3}. \tag{4.4}$$

Using eqs. (4.2) and (4.4), χ_{zz} can be written up to order β^6

$$\begin{aligned}
\chi_{zz} = {} & (\beta/4)\, d_{000} - (\beta/4)^2\, d_{001}J_3 \\
& - (\beta/4)^3\, \tfrac{1}{3}\, [d_{200}\, (J_1^2 + J_2^2) + d_{110}J_1J_2 + d_{002}J_3^2] \\
& + (\beta/4)^4\, \tfrac{1}{3}\, [d_{201}\, (J_1^2 + J_2^2)\, J_3 + d_{111}J_1J_2J_3 + d_{003}J_3^3] \\
& + (\beta/4)^5\, \tfrac{1}{15}\, [d_{400}\, (J_1^4 + J_2^4) + d_{310}\, (J_1^3J_2 + J_1J_2^3) + d_{220}J_1^2J_2^2 \\
& + d_{202}\, (J_1^2 + J_2^2)\, J_3^2 + d_{112}J_1J_2J_3^2 + d_{004}J_3^4] \\
& + (\beta/4)^6\, \tfrac{1}{45}\, [d_{401}\, (J_1^4 + J_2^4)\, J_3 + d_{311}\, (J_1^3J_2 + J_1J_2^3)\, J_3 \\
& + d_{221}J_1^2J_2^2J_3 + d_{203}\, (J_1^2 + J_2^2)\, J_3^3 + d_{113}J_1J_2J_3^3 + d_{005}J_3^5].
\end{aligned} \tag{4.5}$$

Many of the coefficients in eq. (4.5) can be determined from the high-temperature expansion for the transverse susceptibility χ_{xx} of the anisotropic XY model which we have derived in ref. 10. As we have shown there, one has to be careful in replacing the spin-cyclic model by its c-cyclic analogue. In fact, the c-cyclic model will lead to erroneous results, even in the thermodynamic limit, since in the time-dependent correlation functions of the xx components the Jordan-Wigner factors in front of the α and β operators are also time dependent and in this way the local perturbation between the spins N and 1 which arises in the c-cyclic formulation is propagated through the whole chain. Furthermore an exact calculation is not possible and the derivation of a high-temperature expansion is rather tedious.

For the XY model, defined by the hamiltonian

$$\mathscr{H}_{XY} = J_1 \sum_{i=1}^{N} S_i^x S_{i+1}^x + J_2 \sum_{i=1}^{N} S_i^y S_{i+1}^y , \tag{4.6}$$

the transverse susceptibility χ_{xx} up to order β^6 is given by

$$\begin{aligned} \chi_{xx} = {} & \tfrac{1}{4}\beta - (\beta/4)^2\, 2J_1 + (\beta/4)^3\, \tfrac{1}{3}\,(6J_1^2 - 2J_2^2) \\ & + (\beta/4)^4\, \tfrac{1}{3}\,(-4J_1^3 + 6J_1J_2^2) + (\beta/4)^5\, \tfrac{1}{15}\,(10J_1^4 - 32J_1^2J_2^2 + 6J_2^4) \\ & + (\beta/4)^6\, \tfrac{1}{45}\,(-12J_1^5 + 44J_1^3J_2^2 - 66J_2^4J_1) . \end{aligned} \tag{4.7}$$

This expression has been obtained from eq. (5.18) of ref. 10 by substituting $S_{-1} = \frac{1}{2}J_1$, $S_1 = \frac{1}{2}J_2$ and $B = 0$. (The simple cases corresponding to $J_2 = 0$ and $J_1 = 0$ can also be obtained respectively from the susceptibility of the Ising model and the χ_{zz} susceptibility of the XY model.)

By elementary symmetry considerations we can obtain the χ_{zz} component of the susceptibility for the anisotropic Heisenberg model in the special case that $J_2 = 0$. This can be done by the substitution $J_1 \to J_3$, $J_2 \to J_1$ in eq. (4.7). As a result we obtain all coefficients $d_{\nu_1 0 \nu_3}$ with $\nu_1 + \nu_3 \leq 5$, *i.e.*

$$\begin{aligned} & d_{000} = 1, \quad d_{001} = 2, \\ & d_{200} = 2, \quad d_{002} = -6, \quad d_{201} = 6, \quad d_{003} = -4, \\ & d_{400} = 6, \quad d_{202} = -32, \quad d_{004} = 10, \\ & d_{401} = -66, \quad d_{203} = 44, \quad d_{005} = -12. \end{aligned} \tag{4.8}$$

The coefficients $d_{\nu_1\nu_2\nu_3}$ with $\nu_3 = 0, 1$ can be determined by using the first-order perturbation calculation in J_3 treated in section 2. Expanding $\ln z$, for $B \neq 0$, *cf.* eqs. (2.18), (2.21) and (2.22), we have

$$\begin{aligned} \ln z = {} & B^2\, [(\beta/4)^2\, 2 - (\beta/4)^4\, \tfrac{4}{3}\,(J_1^2 + J_2^2 + J_1J_2) \\ & + (\beta/4)^6\, \tfrac{4}{5}\,(J_1^4 + J_2^4 + 2J_1^3J_2 + 2J_1J_2^3 + 4J_1^2J_2^2)] \\ & + B^2J_3\, \{-(\beta/4)^3\, 4 + (\beta/4)^5\, 4\,(J_1^2 + J_2^2) \\ & + (\beta/4)^7\, \tfrac{1}{45}\,[-132\,(J_1^4 + J_2^4) + 104\,(J_1^3J_2 + J_1J_2^3) - 304J_1^2J_2^2]\} \\ & + \text{other terms}, \end{aligned} \tag{4.9}$$

where the other terms are independent of B or proportional to higher powers B^4 and B^6. Using (4.3) and (4.5) we obtain additional relations for the coefficients

$$\begin{aligned} &d_{110} = 2, \quad d_{111} = 0, \quad d_{220} = 24, \quad d_{310} = 12, \\ &d_{311} = 52, \quad d_{221} = -152. \end{aligned} \tag{4.10}$$

So far we have determined all coefficients in eq. (4.5) apart from d_{112} and d_{113}. These coefficients can be determined by using the high-temperature expansion for the isotropic case $J_1 = J_2 = J_3 = J$, *cf.* Baker *et al.*[2]),

$$\begin{aligned} \ln z = B^2\, [(\beta/4)^2\, 2 - (\beta/4)^3\, 4J + (\beta/4)^5\, \tfrac{16}{3} J^3 \\ + (\beta/4)^6\, \tfrac{20}{3} J^4 - (\beta/4)^7\, \tfrac{56}{5} J^5] + \text{other terms}. \end{aligned} \tag{4.11}$$

Eq. (4.11) has been obtained from eq. (3.5) in ref. 2 by substituting $K = -\tfrac{1}{4}\beta J$, $\bar{H} = \tfrac{1}{2}\beta B$.

From eqs. (4.3), (4.5) and (4.11), we have the relations

$$\begin{aligned} &2d_{400} + 2d_{310} + d_{220} + 2d_{202} + d_{112} + d_{004} = 50, \\ &2d_{401} + 2d_{311} + d_{221} + 2d_{203} + d_{113} + d_{005} = -252. \end{aligned} \tag{4.12}$$

By inserting eqs. (4.8) and (4.10), we obtain

$$d_{112} = 44, \quad d_{113} = -148 \tag{4.13}$$

and all coefficients in the expansion of χ_{zz} up to the order β^6 have been determined. The result can be written

$$\begin{aligned} \chi_{zz} = \tfrac{1}{4}\beta - (\beta/4)^2\, 2J_3 - (\beta/4)^3\, \tfrac{2}{3}\, (J_1^2 + J_2^2 + J_1J_2 - 3J_3^2) \\ + (\beta/4)^4\, \tfrac{2}{3}\, [3\, (J_1^2 + J_2^2)\, J_3 - 2J_3^3] \\ + (\beta/4)^5\, \tfrac{2}{15}\, [3\, (J_1^4 + J_2^4) + 6\, (J_1^3J_2 + J_1J_2^3) + 12J_1^2J_2^2 \\ - 16\, (J_1^2 + J_2^2)\, J_3^2 + 22J_1J_2J_3^2 + 5J_3^4] \\ + (\beta/4)^6\, \tfrac{2}{45}\, [-33\, (J_1^4 + J_2^4)\, J_3 + 26\, (J_1^3J_2 + J_1J_2^3)\, J_3 \\ - 76J_1^2J_2^2J_3 + 22\, (J_1^2 + J_2^2)\, J_3^3 - 74J_1J_2J_3^3 - 6J_3^5]. \end{aligned} \tag{4.14}$$

An expansion up to higher orders of β would involve an extension of the expansion of χ_{xx} for the XY model as given in ref. 10. In the present paper we restrict ourselves to the order β^6.

5. Results and discussion

In this section we investigate the behaviour of the specific heat and the susceptibility χ_{zz} for a few values of the coupling constants which are taken either all positive (antiferromagnetic case) or all negative (ferromagnetic case). We shall discuss in particular some characteristic features due to deviations from axial symmetry in the absence of a magnetic field.

First we consider the specific heat per spin using the high-temperature expansion up to order β^9, which can be obtained from (3.13) using the relation

$$c = k\beta^2 \frac{\partial^2 \ln z}{\partial \beta^2}. \tag{5.1}$$

Here we shall restrict ourselves to β values satisfying $0 \leq \beta \leq 1.5$. The region of validity of our high-temperature expansion depends of course on the specific values of the interaction constants. For the values of the interaction constants which we shall consider the expansion is quite accurate. In fact, the numerical agreement between the results of the two expansions (3.13) and (3.14) shows that the term proportional to β^{11} can be neglected. On the other hand, the interval of β is large enough to show some typical effects due to deviations from axial symmetry. Of course, one could pursue the analysis to much higher values of β, by deriving a few more terms in the high-temperature expansion and by performing a Padé-approximent analysis, *cf.* Baker *et al.*[2]). But this is outside the scope of the present paper.

In fig. 1 we have plotted the specific heat c/k *vs.* β for $J_3 = 0.2$ and a few values of J_1 and J_2 satisfying $J_1 + J_2 = 1$. These values are characteristic for an aniso-

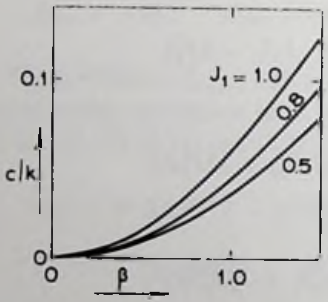

Fig. 1

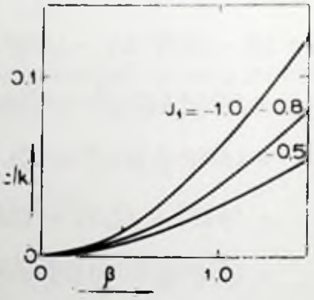

Fig. 2

Fig. 1. The specific heat c/k *vs.* the inverse temperature β for the antiferromagnetic cases: $J_3 = 0.2$; $J_1 = 0{,}5, 0.8, 1.0$; $J_1 + J_2 = 1$.

Fig. 2. The specific heat c/k *vs.* the inverse temperature β for the ferromagnetic cases: $J_3 = -0.2$; $J_1 = -1.0, -0.8, -0.5$; $J_1 + J_2 = -1$.

tropic antiferromagnetic chain with a small exchange interaction between the z components of the spins. The ferromagnetic case with $J_3 = -0.2$ and $J_1 + J_2 = -1$ has been plotted in fig. 2. In both figures we see that the specific heat varies considerably with the deviation $J_1 - J_2$ from axial symmetry, keeping $J_1 + J_2$ fixed. In fact in both figures, the lowest curves of the specific heat correspond to the case of axial symmetry ($J_1 = J_2$). In the high-temperature limit this can be seen from the leading term

$$c \sim k\,(\beta/4)^2\,(J_1^2 + J_2^2 + J_3^2), \tag{5.2}$$

which implies that for small β, the ratio between the specific heat for the anisotropic cases $|J_1| = 0.8$, 1.0 and the specific heat in the axial case $|J_1| = 0.5$ are given by $\frac{4}{3}$ and $\frac{52}{27}$, respectively. For larger values of β, the ratio between the antiferromagnetic specific heats becomes smaller as compared to the numbers given above, whereas in the ferromagnetic case the ratio will be enhanced. Note that for $|J_1| = 1$, the specific heat is invariant under inversion of sign of the interaction constants, as should be the case for an anisotropic XY model. For values of J_1 with $0 < |J_1| < 1$ the antiferromagnetic specific heat in this temperature region is larger than the corresponding ferromagnetic one. (For low temperatures one should expect the opposite situation, *i.e.*, the antiferromagnetic specific heat is smaller than the ferromagnetic one. This can also be shown from spin-wave theory in the isotropic case $J_1 = J_2 = J_3 = J$. In the ferromagnetic case the specific heat is proportional to $T^{\frac{1}{2}}$, whereas in the antiferromagnetic case $c \sim T$, *cf.* refs. 12, 14.)

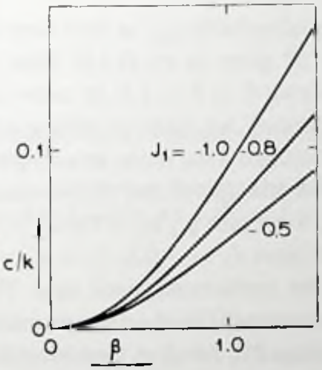

Fig. 3. The specific heat c/k *vs.* the inverse temperature β for the ferromagnetic cases: $J_3 = -0.8$; $J_1 = -1.0, -0.8, -0.5$; $J_1 + J_2 = -1$.

In fig. 3 we have plotted c/k *vs.* β for $J_3 = -0.8$ and a few values of J_1 and J_2 satisfying $J_1 + J_2 = -1$, corresponding to the ferromagnetic case and a large exchange between the z components. Here again the lowest curve corresponds to axial symmetry. In the high-temperature limit the ratios between the specific heat for $J_1 = -0.8, -1.0$ and the specific heat in the axial case $J_1 = -0.5$ are given by $\frac{22}{19}$ and $\frac{82}{57}$, respectively. For increasing values of β the ratios become larger. We have not plotted the specific heat for the corresponding antiferromagnetic case $J_3 = 0.8, J_1 + J_2 = 1$. However, the curve for $J_1 = 1, J_2 = 0, J_3 = 0.8$ coincides exactly with the upper curve in fig. 3. In this case, the deviations from axial symmetry are not important. The c/k values for $\beta = 0.5, 1.0, 1.5$ in the axial case are given by 0.020, 0.078, 0.163, whereas the corresponding values for $\beta = 0.5, 1.0, 1.5$ and $J_1 = 0.8$ and $J_1 = 1.0$ are given by 0.021, 0.082, 0.164 and 0.025, 0.089, 0.167, respectively.

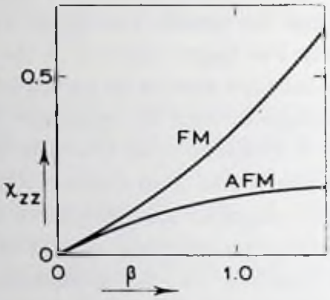

Fig. 4. The susceptibility χ_{zz} *vs.* the inverse temperature β for the antiferromagnetic case (AFM) $J_3 = 0.8, J_1 = J_2 = 0.5$, and for the ferromagnetic case (FM) $J_3 = -0.8, J_1 = J_2 = -0.5$.

We shall now discuss the susceptibility χ_{zz} in field zero using the high-temperature expansion up to order β^6 given in eq. (4.14). Here again we shall restrict ourselves to values of β satisfying $0 \leq \beta \leq 1.5$. In order to discuss the influence of deviations from axial symmetry we have to distinguish between two cases: i) the symmetry axis is parallel to the z axis; ii) the axis of symmetry is perpendicular to the z axis. In the first case we take J_3 fixed and choose various values of J_1 and J_2 keeping $J_1 + J_2$ fixed. In fig. 4 we plot χ_{zz} *vs.* β for $J_3 = 0.8$ and $J_1 = J_2 = 0.5$ and the ferromagnetic counterpart $J_3 = -0.8, J_1 = J_2 = -0.5$. Obviously, the lower curve corresponds to the antiferromagnetic case. The effects due to deviations from axial symmetry are small. In the ferromagnetic case, the deviations in the χ_{zz} values are smaller than 2% for $\beta \leq 1$ and for $\beta = 1.5$ they amount to at most 5% (the χ_{zz} seems to be maximal in the axial case). In the antiferromagnetic case, the deviations are negligible for all values $\beta \leq 1.5$. [Such small deviations can also be found within the XY model, ($J_3 = 0$), *cf.* ref. 10, where χ_{zz} has a very weak dependence on the anisotropy parameter γ.]

In the second case we consider a fixed value of J_1 and choose various values of J_2 and J_3, $J_2 + J_3$ being fixed. In fig. 5 we plot χ_{zz} *vs.* β for $J_1 = -0.8, J_2 + J_3 = -1$.

We see that χ_{zz} increases, if J_3 decreases from 0 to -1. In this case, the deviations from axial symmetry are important and depend also on the sign of the "anisotropy" parameter $J_3 - J_2$.

Finally, in fig. 6, we give χ_{zz} *vs.* β for the antiferromagnetic case, where $J_1 = 0.8$, $J_2 + J_3 = 1$, $J_3 = 0.2$, 0.5, 0.8 and 1.0. We have omitted the special case $J_3 = 0$. In that case the χ_{zz} coincides with the χ_{zz} for $J_3 = 0, J_2 = -1, J_1 = -0.8$ plotted in fig. 5. The antiferromagnetic susceptibility decreases, if J_3 increases from 0 to 1. In the case of axial symmetry we have $J_2 = J_3 = 0.5$. The influence of the deviations from axial symmetry is still large, but somewhat smaller than in the ferromagnetic case.

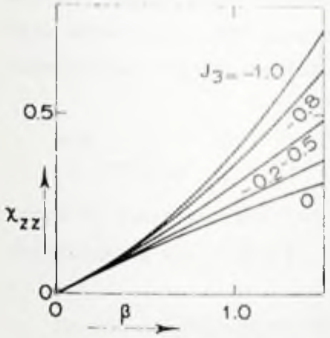

Fig. 5

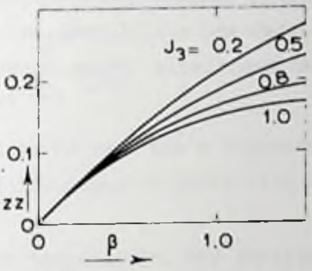

Fig. 6

Fig. 5. The susceptibility χ_{zz} *vs.* the inverse temperature β for the ferromagnetic cases: $J_1 = -0.8$; $J_3 = -1.0, -0.8, -0.5, -0.2, 0.0$; $J_2 + J_3 = -1$.

Fig. 6. The susceptibility χ_{zz} *vs.* the inverse temperature β for the antiferromagnetic cases: $J_1 = 0.8$; $J_3 = 0.2, 0.5, 0.8, 1.0$; $J_2 + J_3 = 1$.

The analysis treated above may be useful for the experimental investigation of anisotropy in one-dimensional spin systems. Many examples of such one-dimensional systems can be found in the review by De Jongh and Miedema[14]). Most of these examples seem to be well described by an isotropic Heisenberg hamiltonian. However, in systems containing transition ions with spin $S \geq 1$, there may be a low-lying Kramers doublet, which can be described in terms of an effective spin $S' = \frac{1}{2}$. Then, in terms of the effective spins, the exchange interaction will in general be anisotropic. A one-dimensional example of such a situation has been described, *e.g.*, by Klaaijsen[15]).

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III. ON THE SUSCEPTIBILITY OF THE ONE-DIMENSIONAL ISING CHAIN

1. Introduction and summary

In recent years one-dimensional magnetic systems have received a great deal of interest. Many experimental data have been given for systems which can be characterized by a large exchange coupling between neighbouring atoms lying on one-dimensional chains (intrachain coupling) and a much smaller exchange coupling between atoms belonging to different chains (interchain coupling). For a review, see de Jongh and Miedema 1). For low temperatures the small interchain coupling can give rise to long-range magnetic ordering and the system behaves essentially as a two- or three-dimensional system. Well above the transition temperature the system has essentially one-dimensional properties and can be described by a hamiltonian of the type

$$\mathcal{H} = \sum_{\alpha=x,y,z} 2J_\alpha \sum_{i=1}^{N} S_i^\alpha S_{i+1}^\alpha - \sum_{\alpha=x,y,z} \sum_{i=1}^{N} b_\alpha S_i^\alpha \qquad (1.1)$$

where J_α characterizes the exchange coupling between the α components of two neighbouring spins $S = \frac{1}{2}$, and $\vec{b}$ is an applied magnetic field with components b_α.

In the neighbourhood of the transition temperature, the physical properties of the system depend on some global characteristics such as dimensionality, the spatial symmetry and the range of the interactions due to universality and scaling 2),3), rather than the details of the interaction parameters. In the high temperature regime, however, the application of a magnetic field can give information on the details of the intrachain interaction.

Unfortunately, not much is known in general on exact solutions of the hamiltonian (1.1) in the presence of a magnetic field. If one of the exchange parameters J , say J_z, vanishes, we have the one-dimensional XY-model. For this model the free energy in the presence of a magnetic field b_z in the z direction, ($b_x = b_y = 0$), has been calculated exactly 4)-7). In the presence of a magnetic field in the x or y direction there are complications. The behaviour of time-dependent xx correlation functions at zero temperature has been studied in ref. 8, a high-temperature expansion of the xx element of the susceptibility tensor χ_{xx} has been given in ref. 9, but the free energy has not been evaluated exactly, so far.

In the case of three nonvanishing interaction parameters, the situation is much more complicated. Exact solutions for the ground state in the absence of a magnetic field have been given by Yang and Yang for the XXZ hamiltonian with $J_x = J_y$ 10) and by Baxter for the general XYZ hamiltonian in which J_x, J_y and J_z are different 11). For a review we refer to refs. 12 and 13.

In the presence of a magnetic field and also for finite temperatures approximate methods have to be used. A high-temperature expansion for the specific heat and the susceptibility χ_{zz} has been given by Baker et al. for the isotropic case with $J_x = J_y = J_z$ 14), and by Dalton and Wood 15) and Jou and Chen 16) for the XXZ hamiltonian. The calculations in refs. 15 and 16 also apply to general lattice systems with axial symmetry.

In a previous paper we have given a high-temperature expansion for the specific heat of the one-dimensional XYZ hamiltonian using first-order perturbation calculation relative to the XY-model 17). Furthermore, finite chain calculations can be extrapolated to give very reliable results on thermodynamic quantities, cf. the paper by Bonner and Fisher 18) on the specific heat and the susceptibility χ_{zz} of the XXZ hamiltonian and a recent paper by Blöte 19) on the specific heat of the XXZ hamiltonian also taking into account the effect of higher spin values $S \geq 1$ and the effect of crystalline fields.

In the present paper we investigate the tensor of the magnetic susceptibility in the presence of a magnetic field $\vec{b}$ in the simple case of the Ising hamiltonian with $J_y = J_z = 0$. The $\alpha\alpha$ element of the susceptibility tensor is given by

$$\chi_{\alpha\alpha}(\vec{b}) = -\lim_{b_\alpha \to 0} \frac{\partial^2 f}{\partial b_\alpha^2} \left[\mathcal{H}_I - \vec{b}\cdot\sum_i \vec{S}_i - b_\alpha \sum_i S_i^\alpha \right] \tag{1.2}$$

where

$$\mathcal{H}_I = 2J \sum_{i=1}^{N} S_i^x S_{i+1}^x , \qquad S_{N+1}^x \equiv S_1^x \tag{1.3}$$

is the Ising hamiltonian with periodic boundary conditions and

$$f[\mathcal{H}] = - \lim_{N\to\infty} (\beta N)^{-1} \ln \langle e^{-\beta\mathcal{H}} \rangle \tag{1.4}$$

is the free energy per particle corresponding to the hamiltonian $\mathcal{H}$ in the thermodynamic limit and

$$\langle A \rangle \equiv \mathrm{Tr}\, A \tag{1.5}$$

for an arbitrary operator A.

$\chi_{\alpha\alpha}$, as defined by (1.2) can also be expressed in terms of correlation functions. In the thermodynamic limit we have

$$\chi_{\alpha\alpha}(\vec{b}) = \int_0^\beta d\tau \, \{ \langle \rho(\vec{b})\, S_1^\alpha(\tau) S_1^\alpha \rangle - \langle \rho(\vec{b}) S_1^\alpha \rangle^2 \} +$$

$$+ 2 \sum_{p=1}^{\infty} \int_0^\beta d\tau \, \{ \langle \rho(\vec{b}) S_1^\alpha(\tau) S_{p+1}^\alpha \rangle - \langle \rho(\vec{b}) S_1^\alpha \rangle \langle \rho(\vec{b}) S_{p+1}^\alpha \rangle \} \tag{1.6}$$

where

$$\rho(\vec{b}) = \left(\exp[-\beta\{\mathcal{H}_I - \vec{b}\cdot\sum_i \vec{S}_i\}]\right) \langle \exp[-\beta\{\mathcal{H}_I - \vec{b}\cdot\sum_i \vec{S}_i\}] \rangle^{-1} \tag{1.7}$$

is the density operator and

$$A(\tau) = \left(\exp[\tau\{\mathcal{H}_I - \vec{b}\cdot\sum_i \vec{S}_i\}]\right) A \left(\exp[-\tau\{\mathcal{H}_I - \vec{b}\cdot\sum_i \vec{S}_i\}]\right) \tag{1.8}$$

for an arbitrary operator A.

Apart from the susceptibility we also investigate the staggered susceptibility which is defined by the relation

$$\chi_{\alpha\alpha}^{s}(\vec{b}) = - \lim_{b_\alpha^s \to 0} \frac{\partial^2 f}{\partial {b_\alpha^s}^2} [\mathcal{H}_I - \vec{b}\cdot\sum_i \vec{S}_i - b_\alpha^s \sum_i (-1)^i S_i^\alpha] \quad . \tag{1.9}$$

Here b_α^s is a staggered magnetic field with opposite values at even and odd sites in the chain. The staggered susceptibility can be important e.g. if one wants to describe antiferromagnetic ordering due to interchain coupling in terms of a molecular field model, see Stout and Chisholm [20] and Nagle and Bonner [21],[22]. This will be discussed in more detail in section 6 of this paper. Furthermore, the staggered susceptibility can also be important in the presence of an antisymmetric exchange term of the Dzyaloshinsky type [23],[24]. This will be shown in a following paper [25]. In terms of correlation functions, $\chi_{\alpha\alpha}^s$ is given by

$$\chi_{\alpha\alpha}^{s}(\vec{b}) = \int_0^\beta d\tau \langle \rho(\vec{b}) S_1^\alpha(\tau) S_1^\alpha \rangle + 2 \sum_{p=1}^{\infty} (-1)^p \int_0^\beta d\tau \langle \rho(\vec{b}) S_1^\alpha(\tau) S_{p+1}^\alpha \rangle \ . \tag{1.10}$$

In the discussion of the susceptibilities we shall distinguish between two cases:

(i) The magnetic field $\vec{b}$ is in the x direction, $\vec{b} = b\vec{e}_x$, parallel to the components of the spins coupled by the Ising interaction. The susceptibilities and the density operator are denoted by

$$\chi_{\alpha\alpha,x} \equiv \chi_{\alpha\alpha}(b\vec{e}_x),\ \chi^{s}_{\alpha\alpha,x} \equiv \chi^{s}_{\alpha\alpha}(b\vec{e}_x),\ \rho_x \equiv \rho(b\vec{e}_x)\ . \tag{1.11}$$

(ii) The magnetic field $\vec{b}$ is in the z direction, $\vec{b} = b\vec{e}_z$, perpendicular to the spin components. The susceptibilities and the density operator are denoted by

$$\chi_{\alpha\alpha,z} \equiv \chi_{\alpha\alpha}(b\vec{e}_z),\ \chi^{s}_{\alpha\alpha,z} \equiv \chi^{s}_{\alpha\alpha}(b\vec{e}_z),\ \ \rho_z \equiv \rho(b\vec{e}_z)\ . \tag{1.12}$$

In section 2 we deal with the susceptibilities $\chi_{\alpha\alpha,x}$ and $\chi^{s}_{\alpha\alpha,x}$ for $\alpha = x,y,z$. In particular the transverse susceptibilities with $\alpha = y,z$ are calculated for all values of the magnetic field $\vec{b} = b\vec{e}_x$. To our knowledge no explicit expression has been given for finite values of b. In section 3 we discuss the yy and zz components of the susceptibility in the presence of a magnetic field $\vec{b} = b\vec{e}_z$, which can be obtained exactly using the theory of the XY-model and the alternating XY-model 26),27). Finally the quantities $\chi_{xx,z}$ and $\chi^{s}_{xx,z}$ in the presence of a magnetic field $\vec{b} = b\vec{e}_z$ cannot be calculated exactly. In section 4 these susceptibilities are evaluated using perturbation calculation for small and large values of the applied field.

In section 5 we investigate the susceptibilities in more detail for small values of the applied magnetic field. As a result the susceptibilities have a minimum for $\vec{b} = 0$ and hence a maximum at some finite value of the applied field for sufficiently low temperature. On the other hand the staggered susceptibilities $\chi^{s}_{xx,x}$, $\chi^{s}_{xx,z}$ and $\chi^{s}_{zz,z}$ show a maximum at $\vec{b} = 0$ for all temperatures.

In section 6 the interchain coupling is investigated in terms of a molecular field model, or more specifically in terms of a model with long-range (separable) interactions, for which the molecular field approximation can be shown to produce rigorous results 28),29). Furthermore, we discuss the relation between the susceptibilities and a curious phenomenon for the phase boundary of the transition from antiferromagnetism to paramagnetism observed by van Tol and Poulis 30),31) in cupric sulphate, using n.m.r. and specific heat measurements. In this substance the critical temperature as a function of the applied magnetic field shows a maximum at a temperature above the Néel temperature corresponding to the transition in zero field.

Assuming that the phase transition is of second order, as has been observed experimentally, the phase boundary can be explained in terms of the properties of the susceptibility of a one-dimensional chain. Although the occurrence of the effect can be explained qualitatively on the basis of a rigorous model, no quantitative agreement can be obtained on the basis of the numerical values of the susceptibility.

2. Susceptibilities of the Ising chain in a parallel field

In order to evaluate the parallel susceptibilities $\chi_{xx,x}$ and $\chi^s_{xx,x}$ in the presence of a magnetic field $b\vec{e}_x$, we consider the hamiltonian

$$\mathcal{H} = 2J \sum_{i=1}^{N} S_i^x S_{i+1}^x - b \sum_{i=1}^{N} S_i^x - b^s \sum_{i=1}^{N} (-1)^i S_i^x \ . \tag{2.1}$$

The free energy per particle has been calculated by Nagle and Bonner 22) using the transfer matrix formalism, cf. e.g. 12),13),32). The partition function $Z \equiv \langle \exp(-\beta\mathcal{H}) \rangle$ can be written

$$Z \equiv \sum_{S_1,\ldots,S_N=\pm\frac{1}{2}} \prod_{i=1}^{N} V_i(S_i,S_{i+1}) = \mathrm{Tr}(V_e V_o)^{\frac{1}{2}N}, \tag{2.2}$$

where

$$V_i(S_i,S_{i+1}) = e^{-2\beta J S_i S_{i+1}} \, e^{\frac{1}{2}\beta b(S_i+S_{i+1})} \, e^{\frac{1}{2}\beta b^s(-1)^i(S_i-S_{i+1})} \tag{2.3}$$

and

$$V_e = V_i, \quad \text{for even values of } i, \quad \text{and}$$
$$V_o = V_i, \quad \text{for odd values of } i \ . \tag{2.4}$$

The free energy per particle is given by

$$f = -\tfrac{1}{2}\beta^{-1} \ln \lambda \tag{2.5}$$

where λ is the largest eigenvalue of the matrix $V_e V_o$, leading to

$$f = -\tfrac{1}{2}\beta^{-1} \ln \Big[e^{-\beta J} \cosh \beta b + e^{\beta J} \cosh \beta b^s + \{ e^{-2\beta J} \sinh^2 \beta b + e^{2\beta J} \sinh^2 \beta b^s + 2 \cosh \beta b \cosh \beta b^s + 2 \}^{\frac{1}{2}} \Big] \ . \tag{2.6}$$

In the homogeneous case with $b^s = 0$, eq. (2.6) reduces to the well-known result 32)

$$f = -\beta^{-1} \ln [e^{-\frac{1}{2}\beta J} \cosh \tfrac{1}{2}\beta b + \{e^{-\beta J} \sinh^2 \tfrac{1}{2}\beta b + e^{\beta J}\}^{\frac{1}{2}}] \, . \tag{2.7}$$

From eq. (2.6) we obtain

$$\chi_{xx,x} = - \lim_{b^s \to 0} \frac{\partial^2 f}{\partial b^2} =$$

$$= \tfrac{1}{4}\beta e^{-\beta J} A^{-\frac{3}{2}} (\cosh \tfrac{1}{2}\beta b) \tag{2.8}$$

and

$$\chi^{s}_{xx,x} = - \lim_{b^s \to 0} \frac{\partial^2 f}{\partial b^{s\,2}} = \tfrac{1}{4}\beta e^{\beta J} A^{-\frac{1}{2}} (\cosh \tfrac{1}{2}\beta b)^{-1} \, , \tag{2.9}$$

where

$$A \equiv 1 + e^{-2\beta J} \sinh^2 \tfrac{1}{2}\beta b \, . \tag{2.10}$$

Transverse susceptibility.

For the transverse susceptibility $\chi_{yy,x}$ in a parallel field, the situation seems to be different. To our knowledge, the transverse susceptibility has been evaluated only for the special case that the parallel field vanishes, as a special case of the XY-model [4)]. The generalization to nonvanishing values of b is straightforward, using eq. (1.6), as we shall show now.

For the operators $S_1^y(\tau)$ and $S_1^z(\tau)$, defined by (1.8) with $\vec{b} = b\vec{e}_x$, we have the equations of motion

$$\frac{d}{d\tau} S_1^y(\tau) = i \, O \, S_1^z(\tau) \quad , \tag{2.11}$$

$$\frac{d}{d\tau} S_1^z(\tau) = - i \, O \, S_1^y(\tau) \tag{2.12}$$

where

$$O \equiv 2J(S_2^x + S_N^x) - b \quad . \tag{2.13}$$

The solution is given by

$$S_1^y(\tau) = S_1^y \cosh O\tau + i\, S_1^z \sinh O\tau,$$
$$S_1^z(\tau) = S_1^z \cosh O\tau - i\, S_1^y \sinh O\tau\ . \qquad (2.14)$$

Noting that

$$\langle \rho_x\, S_1^y S_{p+1}^y \rangle = \langle \rho_x S_1^z S_{p+1}^z \rangle = 0 \quad , \text{ for } p \neq 0 \qquad (2.15)$$

where ρ_x is defined by (1.11) and (1.7), it is obvious that only the autocorrelation function $\langle \rho_x S_1^\alpha(\tau) S_1^\alpha \rangle$ for $\alpha = y,z$ can give nonvanishing contributions to the transverse susceptibilities.

Using (2.14), (2.15), (1.6) and (1.10) we obtain

$$\chi_{yy,x} = \chi_{yy,x}^s = \chi_{zz,x} = \chi_{zz,x}^s \qquad (2.16)$$

where

$$\chi_{yy,x} = \int_0^\beta d\tau\, \langle \rho_x S_1^y(\tau) S_1^y \rangle = \int_0^\beta d\tau \{\tfrac{1}{4} \langle \rho_x \cosh O\tau \rangle + \tfrac{1}{2} \langle \rho_x S_1^x \sinh O\tau \rangle\}. \qquad (2.17)$$

From the relations

$$\cosh 2J\tau S_i^x = \cosh J\tau\ ,$$
$$\sinh 2J\tau S_i^x = 2S_i^x \sinh J\tau, \qquad (2.18)$$

the operators $\cosh O\tau$ and $\sinh O\tau$ can be expressed as

$$\cosh O\tau = \{\cosh^2 J\tau + 4S_2^x S_N^x \sinh^2 J\tau\} \cosh b\tau -$$
$$- (S_2^x + S_N^x) \sinh 2J\tau \sinh b\tau,$$

$$\sinh O\tau = (S_2^x + S_N^x) \sinh 2J\tau \cosh b\tau -$$
$$- \{\cosh^2 J\tau + 4S_2^x S_N^x \sinh^2 J\tau\} \sinh b\tau \qquad (2.19)$$

The autocorrelation function $\langle \rho_x S_1^y(\tau) S_1^y \rangle$ can now be expressed in terms of the correlation functions

$$m \equiv \langle \rho_x S_1^x \rangle \quad , \quad \varepsilon \equiv \langle \rho_x S_1^x S_2^x \rangle \quad ,$$
$$\sigma \equiv \langle \rho_x S_N^x S_2^x \rangle \quad , \quad \nu \equiv \langle \rho_x S_N^x S_1^x S_2^x \rangle\ , \qquad (2.20)$$

i.e. the magnetization per particle, the nearest neighbour and next nearest neighbour correlation function and the correlation function of three neighbouring spins. The result is

$$\langle \rho_x S_1^y(\tau) S_1^y \rangle =$$

$$= \left\{\tfrac{1}{16} - \tfrac{1}{4}m + \tfrac{1}{4}\sigma\right\}\cosh(b+2J)\tau + \left\{\tfrac{1}{16} + \tfrac{1}{4}m + \tfrac{1}{4}\sigma\right\}\cosh(b-2J)\tau +$$

$$+ \left\{-\tfrac{1}{8}m + \tfrac{1}{2}\varepsilon - \tfrac{1}{2}\nu\right\}\sinh(b+2J)\tau + \left\{-\tfrac{1}{8}m - \tfrac{1}{2}\varepsilon - \tfrac{1}{2}\nu\right\}\sinh(b-2J)\tau +$$

$$+ \left(\tfrac{1}{8} - \tfrac{1}{2}\sigma\right)\cosh b\tau + \left(-\tfrac{1}{4}m + \nu\right)\sinh b\tau \ . \tag{2.21}$$

Integrating over τ we find for the susceptibility

$$\chi_{yy,x} =$$

$$= (b+2J)^{-1}\left[\left(\tfrac{1}{16}-\tfrac{1}{4}m+\tfrac{1}{4}\sigma\right)\sinh \beta(b+2J) + \left(-\tfrac{1}{8}m+\tfrac{1}{2}\varepsilon-\tfrac{1}{2}\nu\right)\left\{\cosh \beta(b+2J) - 1\right\}\right] +$$

$$+ (b-2J)^{-1}\left[\left(\tfrac{1}{16}+\tfrac{1}{4}m+\tfrac{1}{4}\sigma\right)\sinh \beta(b-2J) + \left(-\tfrac{1}{8}m-\tfrac{1}{2}\varepsilon-\tfrac{1}{2}\nu\right)\left\{\cosh \beta(b-2J) - 1\right\}\right] +$$

$$+ b^{-1}\left[\left(\tfrac{1}{8}-\tfrac{1}{2}\sigma\right)\sinh \beta b + \left(-\tfrac{1}{4}m+\nu\right)\left(\cosh\beta b - 1\right)\right] \ . \tag{2.22}$$

The correlation functions (2.20) can be calculated in various ways, cf. 13),32),35). For our purpose it is sufficient to consider the probability $P(S_1,S_2,S_3)$ that three adiacent spins S_1^x, S_2^x, S_3^x have the values S_1,S_2,S_3 where S_1, S_2, $S_3 = \pm\frac{1}{2}$. Using the simple relation

$$P(S_1, \tfrac{1}{2}, S_3) = e^{\beta(b-2S_1-2S_3)}\ P(S_1, -\tfrac{1}{2}, S_3) \tag{2.23}$$

we can express σ and ν in terms of ε and m. As a result σ and ν are given by

$$\sigma = \sum_{S_1,S_2,S_3=\pm\frac{1}{2}} S_1S_3\ P(S_1,S_2,S_3) =$$

$$= \tfrac{1}{4}\left(1-e^{-2\beta J}\right)^{-1}\left[e^{\beta(b-2J)}-e^{-\beta b}-4\varepsilon\left(1+e^{-\beta b}+e^{-2\beta J}+e^{\beta(b-2J)}\right) - 4m\left(1+e^{-\beta b}\right)\right] \tag{2.24}$$

and

$$\nu = \sum_{S_1,S_2,S_3=\pm\frac{1}{2}} S_1S_2S_3\ P(S_1,S_2,S_3) =$$

$$= \tfrac{1}{8}\left(1-e^{-2\beta J}\right)^{-1}\Big[-1+e^{-\beta b}-e^{-2\beta J}+e^{\beta(b-2J)} - 4\varepsilon\left(1-e^{-\beta b}-e^{-2\beta J}+e^{\beta(b-2J)}\right) -$$

$$- 2m\left(1-2e^{-\beta b}+e^{-2\beta J}\right)\Big] \ . \tag{2.25}$$

ε and m can be obtained directly from eq. (2.7), i.e.

$$\varepsilon = \tfrac{1}{2}\frac{\partial f}{\partial J} = \tfrac{1}{4} - \tfrac{1}{2}A^{-\frac{1}{2}}\{e^{-\beta J}\cosh\tfrac{1}{2}\beta b + A^{\frac{1}{2}}\}^{-1} , \qquad (2.26)$$

$$m = -\frac{\partial f}{\partial b} = \tfrac{1}{2}A^{-\frac{1}{2}}e^{-\beta J}\sinh\tfrac{1}{2}\beta b , \qquad (2.27)$$

where A has been defined by eq. (2.10).

Hence we have calculated the transverse susceptibilities in the presence of a parallel field $b\vec{e}_x$. In the limit $b \to 0$ eq. (2.22) together with eqs. (2.24) - (2.27) reduces to the familiar result [4)]

$$\chi_{yy} = \frac{\tanh\frac{1}{2}\beta J}{4J} + \frac{\beta}{8\cosh^2\frac{1}{2}\beta J} . \qquad (2.28)$$

3. Transverse susceptibilities in a perpendicular field

In this section we evaluate the susceptibilities $\chi_{yy,z}$, $\chi^s_{yy,z}$, $\chi_{zz,z}$ and $\chi^s_{zz,z}$ in the presence of a magnetic field $b\vec{e}_z$ in the z direction. For the nonstaggered susceptibilities we consider the hamiltonian

$$\mathcal{H} = 2J\sum_{i=1}^{N} S^x_i S^x_{i+1} - b_y\sum_{i=1}^{N} S^y_i - b_z\sum_{i=1}^{N} S^z_i . \qquad (3.1)$$

Note that eq. (3.1) represents the hamiltonian of an Ising chain in a perpendicular magnetic field $b = \sqrt{b_y^2 + b_z^2}$.

The free energy per particle can be evaluated as a special case of the XY-model with anisotropy parameter $\gamma = 1$, cf. refs. [4),6),7)]. The result is

$$f = -(\pi\beta)^{-1}\int_0^{\pi} dq\, \ln 2\cosh\tfrac{1}{2}\beta\Lambda(q) \qquad (3.2)$$

where

$$\Lambda(q) = (J^2 - 2bJ\cos q + b^2)^{\frac{1}{2}} \qquad (3.3)$$

and

$$b^2 = b_y^2 + b_z^2 . \qquad (3.4)$$

For $b_y = 0$, we have

$$\frac{\partial\Lambda}{\partial b_y} = 0, \qquad \frac{\partial^2\Lambda}{\partial b_y^2} = \frac{1}{b}\frac{\partial\Lambda}{\partial b} \qquad (3.5)$$

so that

$$\chi_{yy,z} = - \lim_{b_y \to 0} \frac{\partial^2 f}{\partial b_y^2} =$$

$$= \frac{1}{2\pi} \int_0^\pi dq \, \frac{\tanh \frac{1}{2}\beta(J^2-2bJ\cos q + b^2)^{\frac{1}{2}}}{(J^2-2bJ\cos q + b^2)^{\frac{1}{2}}} \left(1 - \frac{J}{b}\cos q\right) = b^{-1} m_z \quad (3.6)$$

where m_z is the magnetization per particle of an Ising chain in the presence of a transverse magnetic field $b\vec{e}_z$.

The zz-susceptibility is given by

$$\chi_{zz,z} = - \lim_{b_y \to 0} \frac{\partial^2 f}{\partial b_z^2} = \frac{1}{2\pi} \int_0^\pi dq \, \frac{\tanh \frac{1}{2}\beta(J^2-2bJ\cos q + b^2)^{\frac{1}{2}}}{(J^2-2bJ\cos q + b^2)^{\frac{3}{2}}} J^2 \sin^2 q \, +$$

$$+ \frac{\beta}{4\pi} \int_0^\pi dq \, \frac{(b - J\cos q)^2}{(J^2-2bJ\cos q + b^2)\cosh^2 \frac{1}{2}\beta(J^2-2bJ\cos q + b^2)^{\frac{1}{2}}} \, . \quad (3.7)$$

Now we shall calculate the staggered susceptibilities. In view of eqs. (1.6) and (1.10) and the relation

$$\int_0^\beta d\tau \, \langle \rho_z S_1^y(\tau) S_{p+1}^y \rangle = 0, \qquad \text{for } p \neq 0 \quad (3.8)$$

which will be proved in appendix A, we have

$$\chi_{yy,z} = \chi_{yy,z}^{s} = \int_0^\beta d\tau \, \langle \rho_z S_1^y(\tau) S_1^y \rangle \, . \quad (3.9)$$

Eq. (3.9) has the following consequence. Consider the Fourier transform $\hat{m}_q$ of the magnetization in the y direction per particle, due to an inhomogeneous magnetic field in the y direction, defined by

$$\hat{m}_q \equiv N^{-1} \sum_j \langle S_j^y \exp[-\beta(\mathcal{H}_I - b_z \sum_i S_i^z - \sum_i b_{yi} S_i^y)] \rangle e^{iqj} .$$

$$\cdot \, \langle \exp[-\beta(\mathcal{H}_I - b_z \sum_i S_i^z - \sum_i b_{yi} S_i^y)] \rangle^{-1} \, . \quad (3.10)$$

In a first order perturbation calculation in terms of the inhomogeneous magnetic field b_{yi}, $\hat{m}_q$ is given by

$$\hat{m}_q = \chi(q) \hat{b}_q \quad (3.11)$$

where

$$\hat{b}_q = \sum_j b_{yj}\, e^{iqj} \tag{3.12}$$

is the Fourier transform of the inhomogeneous magnetic field and $\chi(q)$ is the wave number dependent susceptibility defined by

$$\chi(q) = \sum_{p=-\infty}^{+\infty} \int_0^\beta d\tau\, \langle \rho_z S_1^y(\tau) S_{p+1}^y \rangle\, e^{iqp} \quad . \tag{3.13}$$

In view of eq. (3.8), $\chi(q)$ is independent of q, i.e.

$$\chi(q) = \chi_{yy,z} \; . \tag{3.14}$$

This is also true for the transverse susceptibilities in the presence of a magnetic field $\vec{b} = b\vec{e}_x$, cf. eqs. (2.15) and (2.16).

We finally consider the staggered susceptibility $\chi^s_{zz,z}$. This quantity can be obtained from the free energy per particle for an alternating XY-chain, in the presence of an alternating magnetic field in the z direction 26),27). Earlier treatments of an alternating XY-chain do not include an external field 33) or are restricted to the isotropic case 34). Consider as a special case of the treatment in refs. 26 and 27 the hamiltonian

$$\mathcal{H} = 2J \sum_{i=1}^{N} S_i^x S_{i+1}^x - b \sum_{i=1}^{N} S_i^z - b^s \sum_{i=1}^{N} (-1)^i S_i^z \quad . \tag{3.15}$$

Then the free energy per particle is given by

$$f = -(\pi\beta)^{-1} \int_0^{\pi/2} dq \left[\ln\left(2 \cosh\tfrac{1}{2}\beta\{c_2 + (c_2^2 - c_4)^{\frac{1}{2}}\}^{\frac{1}{2}} \right) + \ln\left(2 \cosh\tfrac{1}{2}\beta\{c_2 - (c_2^2 - c_4)^{\frac{1}{2}}\}^{\frac{1}{2}} \right) \right] \tag{3.16}$$

where

$$c_2 = b^2 + b^{s^2} + J^2 \quad ,$$

$$c_4 = (b^2 - b^{s^2})^2 - 2J^2(b^2 - b^{s^2})\cos 2q + J^4 \; . \tag{3.17}$$

Noting that for $b^s = 0$

$$\frac{\partial c_2}{\partial b^s} = \frac{\partial c_4}{\partial b^s} = 0, \quad \frac{\partial^2 c_2}{\partial b^{s\,2}} = 2, \quad \frac{\partial^2 c_4}{\partial b^{s\,2}} = -4b^2 + 4J^2 \cos 2q \; , \tag{3.18}$$

the staggered susceptibility $\chi^{s}_{zz,z}$ is given by

$$\chi^{s}_{zz,z} = \frac{1}{2\pi} \int_0^{\pi} dq \, \frac{\tanh \tfrac{1}{2}\beta\{J^2 - 2|bJ|\cos q + b^2\}^{\frac{1}{2}}}{\{J^2 - 2|bJ|\cos q + b^2\}^{\frac{1}{2}}} \cdot \left\{1 - \frac{b^2 + J^2 \sin^2 q}{|bJ|\cos q}\right\} . \quad (3.19)$$

The integral from 0 to π at the right-hand side of (3.19) can be decomposed into an integral from 0 to $\frac{1}{2}\pi$ which arises from the second term at the right-hand side of (3.16) and an integral from $\frac{1}{2}\pi$ to π, which arises from the first term.

4. Parallel susceptibility in a perpendicular field

In this section we consider the correlation functions

$$\langle \rho_z S^x_1(\tau) S^x_{p+1} \rangle = \frac{\langle (\exp[-(\beta-\tau)(\mathcal{H}_I - b\Sigma_i S^z_i)])\, S^x_1 (\exp[-\tau(\mathcal{H}_I - b\Sigma_i S^z_i)])\, S^x_{p+1} \rangle}{\langle \exp[-\beta(\mathcal{H}_I - b\Sigma_i S^z_i)] \rangle} , \quad (4.1)$$

in the presence of a magnetic field $b\vec{e}_z$ in the z direction, where ρ_z and $\mathcal{H}_I$ are defined by (1.12) and (1.13) respectively. Unfortunately, these correlation functions cannot be evaluated exactly for arbitrary values of b. Therefore we shall use the Dyson perturbation expansion

$$\exp[-\beta(\mathcal{H}_0 + \mathcal{H}_1)] = \exp[-\beta\mathcal{H}_0] \left[1 + \sum_{q=1}^{\infty} (-1)^q \int_0^{\beta} d\tau_1 \int_0^{\tau_1} d\tau_2 \ldots \int_0^{\tau_{q-1}} d\tau_q \prod_{k=1}^{q} \mathcal{H}_1[\tau_k] \right] \quad (4.2)$$

where

$$A[\tau] \equiv \left(\exp[\tau\mathcal{H}_0]\right) A \left(\exp -[\tau\mathcal{H}_0]\right) \quad (4.3)$$

for an arbitrary operator A.

For small values of b, we take

$$\mathcal{H}_0 = \mathcal{H}_I \; , \quad \rho_I \equiv \exp[-\beta\mathcal{H}_I] \langle \exp[-\beta\mathcal{H}_I] \rangle^{-1} \; , \quad \mathcal{H}_1 = - b \sum_{i=1}^{N} S^z_i \; . \quad (4.4)$$

Using trivial properties like $S^x_i[\tau] = S^x_i$, $\langle \rho_I A[\tau'] B[\tau''] \rangle = \langle \rho_I A[\tau' - \tau''] B \rangle$ and $\langle \rho_I \mathcal{H}_1 \rangle = 0$, the correlation functions up to the order b^2 are given by

$$\langle \rho_z S_1^x(\tau) S_{p+1}^x \rangle = \langle \rho_I S_1^x S_{p+1}^x \rangle +$$

$$+ b^2 \sum_{k,\ell=1}^{N} \left[\begin{array}{l} I_1 \{ \langle \rho_I (S_k^z[\tau_1-\tau_2] S_\ell^z S_1^x S_{p+1}^x - S_k^z[\tau_1-\tau_2] S_\ell^z \langle \rho_I S_1^x S_{p+1}^x \rangle)) \rangle \} + \\ + I_2 \{ \langle \rho_I (S_1^x S_k^z[\tau_1-\tau_2] S_\ell^z S_{p+1}^x - S_k^z[\tau_1-\tau_2] S_\ell^z \langle \rho_I S_1^x S_{p+1}^x \rangle)) \rangle \} + \\ + I_3 \{ \langle \rho_I (S_k^z[\tau_1-\tau_2] S_1^x S_\ell^z S_{p+1}^x - S_k^z[\tau_1-\tau_2] S_\ell^z \langle \rho_I S_1^x S_{p+1}^x \rangle)) \rangle \} \end{array} \right] \tag{4.5}$$

where the integrations I_1, I_2, I_3 are defined by

$$I_1 = \int_\tau^\beta d\tau_1 \int_\tau^{\tau_1} d\tau_2 , \qquad I_2 \equiv \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 , \qquad I_3 \equiv \int_\tau^\beta d\tau_1 \int_0^\tau d\tau_2 . \tag{4.6}$$

The terms proportional to $b^2 \langle \rho_I S_1^x S_{p+1}^x \rangle$ arise from the denominator in (4.1), as can be seen from the trivial identity

$$I_1 + I_2 + I_3 = \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 . \tag{4.7}$$

Eq. (4.5) has the advantage that no terms proportional to N occur at the right-hand side in view of the cancellation of these terms in the numerator and denominator of (4.1). Using eqs. (2.14) and (2.19), we have in the special case that $b = 0$,

$$S_k^z[\tau] = S_k^z \cosh^2 J\tau + 4 S_k^z S_{k-1}^x S_{k+1}^x \sinh^2 J\tau - i (S_k^y S_{k+1}^x + S_k^y S_{k-1}^x) \sinh 2J\tau . \tag{4.8}$$

From the expression

$$\rho_I = 2^{-N} \prod_{k=1}^{N} (1 - 4 S_k^x S_{k+1}^x \tanh \tfrac{1}{2}\beta J) , \tag{4.9}$$

which can be derived in the thermodynamic limit using similar arguments as in the high temperature expansion [32], it is clear that only terms with $k = \ell$ can give a nonvanishing contribution to $\langle \rho_z S_1^x(\tau) S_{p+1}^x \rangle$. Consider therefore an arbitrary term with $k \neq \ell$ at the right-hand side of eq. (4.5). Inserting the right-hand side of eq. (4.8) we are left with a correlation function which is linear in the operator S_k^y or the operator S_k^z. Such a correlation function must vanish, as is clear taking the trace over the Hilbert space of spin k.

Using eq. (4.8) and the (anti)commutation relations of the spins by which the remaining operators S^y and S^z can be expressed in terms of components S^x, the correlation functions can be written as

$$\begin{aligned}
\langle \rho_z S_1^x(\tau) S_{p+1}^x \rangle = {} & \langle \rho_I S_1^x S_{p+1}^x \rangle + \\
& + b^2 \sum_{k=1}^{N} \left\{ \langle \rho_I S_{k-1}^x S_{k+1}^x S_1^x S_{p+1}^x \rangle - \langle \rho_I S_{k-1}^x S_{k+1}^x \rangle \langle \rho_I S_1^x S_{p+1}^x \rangle \right\} \cdot \\
& \cdot (I_1 + I_2 + I_3) \sinh^2 J(\tau_1 - \tau_2) + \\
& + b^2 \sum_{k=1}^{N} \left\{ \langle \rho_I S_k^x S_{k+1}^x S_1^x S_{p+1}^x \rangle - \langle \rho_I S_k^x S_{k+1}^x \rangle \langle \rho_I S_1^x S_{p+1}^x \rangle \right\} \cdot \\
& \cdot (I_1 + I_2 + I_3) \sinh 2J(\tau_1 - \tau_2) - \\
& - b^2 \Big\{ \tfrac{1}{2} \langle \rho_I S_1^x S_{p+1}^x \rangle I_3 \cosh^2 J(\tau_1 - \tau_2) + 2 \langle \rho_I S_N^x S_1^x S_2^x S_{p+1}^x \rangle I_3 \sinh^2 J(\tau_1 - \tau_2) + \\
& + \tfrac{1}{4} \left(\langle \rho_I S_2^x S_{p+1}^x \rangle + \langle \rho_I S_N^x S_{p+1}^x \rangle \right) \quad I_3 \sinh 2J(\tau_1 - \tau_2) \Big\} .
\end{aligned} \tag{4.10}$$

In this way the correlation functions $\langle \rho_z S_1^x(\tau) S_{p+1}^x \rangle$ have been expressed in terms of integrals multiplied by static correlation functions of two and four spins of the one-dimensional Ising model. The static correlations are given by

$$\langle \rho_I \prod_{k=1}^{n} S_{i_k}^x S_{j_k}^x \rangle = \prod_{k=1}^{n} \tfrac{1}{4}(-T)^{j_k - i_k} ,$$

$$j_k > i_k , \qquad i_{k+1} > j_k , \qquad T \equiv \tanh \tfrac{1}{2}\beta J \tag{4.11}$$

which is obvious from (4.9), since only the term which contains $S_{i_1}^x S_{j_1}^x , \ldots S_{i_n}^x S_{j_n}^x$ once and the intermediate spins between i_k and j_k twice can give a nonvanishing contribution in the thermodynamic limit. Using the explicit expressions of the correlation functions and the integrals in eq. (4.10), which have been listed in appendix B, the correlation functions are given by

$$\begin{aligned}
\langle \rho_z S_1^x(\tau) S_1^x \rangle = {} & \tfrac{1}{4} + \tfrac{1}{16} b^2 J^{-2} \Big[- (\beta - \tau)\tau J^2 (1 - T^2) - \tfrac{1}{4}(1 + T^2) + \\
& + \tfrac{1}{8}\{ e^{(2\beta - 2\tau)J} + e^{2\tau J} - e^{2\beta J} \}(1 - T)^2 + \tfrac{1}{8}\{ e^{-(2\beta - 2\tau)J} + e^{-2\tau J} - e^{-2\beta J} \}(1 + T)^2 \Big] ,
\end{aligned} \tag{4.12}$$

$$\langle \rho_z S_1^x(\tau) S_{p+1}^x \rangle = \tfrac{1}{4}(-T)^p + \tfrac{1}{16} b^2 J^{-2} \cdot$$

$$\cdot \Big[\tfrac{1}{8}(-T)^{p-1} \{4T + (e^{(2\beta-2\tau)J} + e^{2\tau J} - e^{2\beta J})(1-T)^2 -$$

$$- (e^{-(2\beta+2\tau)J} + e^{-2\tau J} - e^{-2\beta J})(1+T)^2 + p(-4\beta J + e^{2\beta J} - e^{-2\beta J})(1-T^2)\} +$$

$$+ \tfrac{1}{16}(-T)^{p-2}\{p-1 + 2T^2 - (p+1)T^4\}\{-4\beta^2 J^2 + e^{2\beta J} + e^{-2\beta J} - 2\}\Big], \quad p \neq 0. \tag{4.13}$$

The xx susceptibility $\chi_{xx,z}$ can now be evaluated, using eq. (1.6) and performing the integration over τ. The result is

$$\chi_{xx,z} = \tfrac{1}{4}\beta e^{-\beta J} + a_{xx,z}(\beta,J) b^2 \tag{4.14}$$

where

$$a_{xx,z}(\beta,J) = \tfrac{1}{256}(J^3 \cosh^4 \tfrac{1}{2}\beta J)^{-1} \cdot$$

$$\cdot \Big[- \tfrac{4}{3}(\beta J)^3(1 + \cosh \beta J) + 2 \sinh 2\beta J + 4 \sinh \beta J -$$

$$- e^{-\beta J}\{(2\beta J)^2(\cosh 2\beta J + 4 \cosh \beta J + 3) +$$

$$+ [(\beta J)^3 + (\beta J)](4 \cosh \beta J - 4 \sinh \beta J - 2 \sinh 2\beta J + 4)\}\Big] . \tag{4.15}$$

The staggered susceptibility can be evaluated using (1.10). The result is

$$\chi_{xx,z}^s = \tfrac{1}{4} \beta e^{\beta J} + a_{xx,z}^s(\beta,J) b^2 \tag{4.16}$$

where

$$a_{xx,z}^s(\beta,J) = a_{xx,z}(\beta,-J) . \tag{4.17}$$

Eq. (4.17) is also obvious from eq. (4.14) if one applies the transformation $R = \Pi_{k=\mathrm{odd}} \exp(i\pi S_k^z)$, which consists of rotations over π around the z axis at the odd lattice sites and the identical transformation at the even lattice sites. Then

$$R\{2J \sum_i S_i^x S_{i+1}^x - b_x^s \sum_i S_i^x (-1)^i - b \sum_i S_i^z\} R^{-1} =$$

$$= -2J \sum_i S_i^x S_{i+1}^x - b_x^s \sum_i S_i^x - b \sum_i S_i^z \tag{4.18}$$

and for the free energy per particle, we have

$$f\left[2J\sum_i S_i^x S_{i+1}^x - b_x^s\sum_i S_i^x(-1)^i - b\sum_i S_i^z\right] =$$

$$= f\left[-2J\sum_i S_i^x S_{i+1}^x - b_x^s\sum_i S_i^x - b\sum_i S_i^z\right] \; . \tag{4.19}$$

Eq. (4.15) can also be found expanding eq. (2.22) for $\chi_{yy,x}$ and also the correlations σ, ν, ε and m, cf. (2.24) - (2.27) for small values of b, i.e. from the coefficient $a_{yy,x}$ in the relation

$$\chi_{yy,z} = \frac{\tanh\frac{1}{2}\beta J}{4J} + \frac{\beta}{8\cosh^2\frac{1}{2}\beta J} + a_{yy,x}(\beta,J)b^2 + \ldots \tag{4.20}$$

This is obvious, since

$$a_{yy,x}(\beta,J) = -\lim_{b_x\to0,b_y\to0}\frac{1}{2}\frac{\partial^4}{\partial^2 b_x\partial^2 b_y} f\left[\mathcal{H}_I - b_x\sum_i S_i^x - b_y\sum_i S_i^y\right] =$$

$$= -\lim_{b_x\to0,b_z\to0}\frac{1}{2}\frac{\partial^4}{\partial^2 b_x\partial^2 b_z} f\left[\mathcal{H}_I - b_x\sum_i S_i^x - b_z\sum_i S_i^z\right] = a_{xx,z}(\beta,J). \tag{4.21}$$

In this section however, we have given a more detailed perturbation calculation of all correlation functions $\langle\rho_z S_1^x(\tau)S_{p+1}^x\rangle$, since more general results such as e.g. the wave-number dependent susceptibility can be obtained from the correlation functions. Moreover, the methods used in this section can also be applied to higher orders of perturbation, which can lead to explicit expressions for the coefficients of higher powers b^4, b^6, ... in the expansion of $\chi_{xx,z}$.

For large values of the magnetic field we can apply the Dyson expansion (4.2) with $\mathcal{H}_0 = -b\Sigma_i S_i^z$ and $\mathcal{H}_1 = \mathcal{H}_I$. Up to the first order in J, the correlation functions are given by

$$\langle\rho_z S_1^x(\tau)S_{p+1}^x\rangle = \langle\rho_b S_1^x[\tau]S_{p+1}^x\rangle -$$

$$-2J\int_0^{\beta-\tau} d\tau_1\,\langle\rho_b\sum_{k=1}^N S_k^x[\tau+\tau_1]S_{k+1}^x[\tau+\tau_1]S_1^x[\tau]S_{p+1}^x\rangle -$$

$$-2J\int_0^{\tau} d\tau_2\,\langle\rho_b\sum_{k=1}^N S_1^x[\tau]S_k^x[\tau_2]S_{k+1}^x[\tau_2]S_{p+1}^x\rangle \; , \tag{4.22}$$

where

$$A[\tau] = \exp[-\tau b \sum_i S_i^z]\, A \exp[\tau b \sum_i S_i^z] \quad ,$$

$$\rho_b = \exp[\ \beta b \sum_i S_i^z]\ \langle \exp[\beta b \sum_i S_i^z] \rangle^{-1} \tag{4.23}$$

Using the relations

$$S_k^x[\tau] = S_k^x \cosh b\tau - iS_k^y \sinh b\tau \tag{4.24}$$

and

$$\rho_b = 2^{-N} \prod_{k=1}^{N} (1 + 2S_k^z \tanh \tfrac{1}{2}\beta b), \tag{4.25}$$

the correlation functions up to the order J can be written

$$\langle \rho_z S_1^x(\tau) S_1^x \rangle = \frac{1}{8 \cosh^2 \frac{1}{2}\beta b} \cdot [\cosh b(\beta-\tau) + \cosh b\tau] \quad , \tag{4.26}$$

$$\langle \rho_z S_1^x(\tau) S_2^x \rangle = -\left(\frac{J}{16 \cosh^2 \frac{1}{2}\beta b} \right) \cdot$$

$$\cdot \left[\tau \cosh(\beta-\tau)b + (\beta-\tau)\cosh \tau b + \frac{1}{b} \left\{ \sinh(\beta-\tau)b + \sinh \tau b \right\} \right], \tag{4.27}$$

$$\langle \rho_z S_1^x(\tau) S_{p+1}^x \rangle = 0 \quad , \qquad p \geq 2 \ . \tag{4.28}$$

The susceptibility and the staggered susceptibility can be found using eqs. (1.6) and (1.10). The result is

$$\chi_{xx,z} = \frac{\tanh \frac{1}{2}\beta b}{2b} - \frac{J}{b^2} (\tanh \tfrac{1}{2}\beta b)^2 + \mathcal{O}\left(\frac{J^2}{b^3}\right) \tag{4.29}$$

$$\chi_{xx,z}^{s} = \frac{\tanh \frac{1}{2}\beta b}{2b} + \frac{J}{b^2} (\tanh \tfrac{1}{2}\beta b)^2 + \mathcal{O}\left(\frac{J^2}{b^3}\right) \quad . \tag{4.30}$$

5. Results and discussion

In this section we discuss the behaviour of the susceptibilities as defined by eqs. (1.11) and (1.12), up to the second order in the applied magnetic field b. For parallel fields $\vec{b} = b\vec{e}_x$ we define

$$\chi_{\alpha\alpha,x} = \chi_\alpha + a_{\alpha\alpha,x}(\beta,J)b^2 ,$$

$$\chi^s_{\alpha\alpha,x} = \chi^s_\alpha + a^s_{\alpha\alpha,x}(\beta,J)b^2 \qquad (5.1)$$

and in the case of perpendicular fields $\vec{b} = b\vec{e}_z$

$$\chi_{\alpha\alpha,z} = \chi_\alpha + a_{\alpha\alpha,z}(\beta,J)b^2$$

$$\chi^s_{\alpha\alpha,z} = \chi^s_\alpha + a^s_{\alpha\alpha,z}(\beta,J)b^2 . \qquad (5.2)$$

Here χ_α and χ^s_α can be expressed in terms of the parallel and transverse susceptibility of the Ising chain

$$\chi_x = \tfrac{1}{4}\beta e^{-\beta J} , \qquad \chi^s_x = \tfrac{1}{4}\beta e^{\beta J} \qquad (5.3)$$

and

$$\chi_y = \chi^s_y = \chi_z = \chi^s_z = \frac{\tanh \frac{1}{2}\beta J}{4J} + \frac{\beta}{8 \cosh^2 \frac{1}{2}\beta J} . \qquad (5.4)$$

The coefficients a can be expressed in terms of six independent parameters $a_\nu(\beta,J)$ and $a^s_\nu(\beta,J)$, $\nu = 1,2,3$. The first three of these parameters occur in the expansion for the free energy per particle of an Ising chain with xx interactions in the presence of an applied magnetic field $\vec{b} \equiv b_x\vec{e}_x + b_y\vec{e}_y + b_z\vec{e}_z$ up to the order b^4:

$$f = -\beta^{-1} \ln 2 \cosh \tfrac{1}{2}\beta J - \tfrac{1}{8}b_x^2 \beta e^{-\beta J} - (b_y^2+b_z^2)\left[\frac{\tanh \frac{1}{2}\beta J}{8J} + \frac{\beta}{16 \cosh^2 \frac{1}{2}\beta J}\right] -$$

$$- \tfrac{1}{12} a_1(\beta,J)b_x^4 - \tfrac{1}{12} a_2(\beta,J)[b_y^4+b_z^4+6b_y^2b_z^2] - \tfrac{1}{4}a_3(\beta,J)[2b_x^2b_y^2+2b_x^2b_z^2] . \qquad (5.5)$$

Using eqs. (2.16), (3.9) and (5.5) all coefficients except $a^s_{xx,x}$, $a^s_{zz,z}$ and $a^s_{xx,z}$ can be expressed in terms of $a_\nu(\beta,J)$, i.e.

$$a_1(\beta,J) = a_{xx,x} ,$$

$$a_2(\beta,J) = a_{zz,z} = 3a_{yy,z} = 3a^s_{yy,z} ,$$

$$a_3(\beta,J) = a_{yy,x} = a^s_{yy,x} = a_{zz,x} = a^s_{zz,x} = a_{xx,z} . \qquad (5.6)$$

The remaining coefficients $a^s_\nu(\beta,J)$ are defined by

$$a^s_1(\beta,J) = a^s_{xx,x} ,$$

$$a^s_2(\beta,J) = a^s_{zz,z} ,$$

$$a^s_3(\beta,J) = a^s_{xx,z} . \qquad (5.7)$$

The coefficients $a_1(\beta,J)$ and $a_1^s(\beta,J)$ can be evaluated, expanding eqs. (2.8) and (2.9) for small values of b. The result is

$$a_1(\beta,J) = \frac{1}{32}\beta^3(-3e^{-3\beta J} + e^{-\beta J}) \quad ,$$

$$a_1^s(\beta,J) = -\frac{1}{16}\beta^3 \cosh \beta J \quad . \tag{5.8}$$

The coefficients $a_2(\beta,J)$ and $a_2^s(\beta,J)$ can be found from eq. (3.6) or (3.7) and eq. (3.19) and are equal to

$$a_2(\beta,J) = -\frac{1}{128}(J^3\cosh^4\tfrac{1}{2}\beta J)^{-1} \cdot$$
$$\cdot \left[(\beta J)^3(-\cosh\beta J + 2) + 2(\beta J)^2 \sinh \beta J + (\beta J)(\cosh\beta J + 1) - \tfrac{1}{2}\sinh 2\beta J - \sinh \beta J\right],$$

$$a_2^s(\beta,J) = \frac{1}{128}(J^3\cosh^4\tfrac{1}{2}\beta J)^{-1} \cdot$$
$$\cdot \left[\tfrac{1}{3}(\beta J)^3(\cosh\beta J - 2) - 6(\beta J)^2\sinh\beta J + 5(\beta J)(\cosh\beta J + 1) - \tfrac{5}{2}\sinh 2\beta J - 5\sinh\beta J\right]. \tag{5.9}$$

The coefficients $a_3(\beta,J)$ and $a_3^s(\beta,J)$ are given by eqs. (4.15) and (4.17), cf. (5.6) and (5.7).

We now discuss the different coefficients occurring in eqs. (5.1) and (5.2). Here we shall restrict ourselves to the value $J = 1$, which corresponds to an antiferromagnetic exchange interaction. The ferromagnetic case with $J < 0$ can be discussed in a similar way; the coefficients $a_1^s(\beta,J)$, $a_2(\beta,J)$ and $a_2^s(\beta,J)$ are invariant for the change in sign $J \to -J$, whereas $a_3(\beta,-J) = a_3^s(\beta,J)$.

The parallel susceptibility χ_x for $J = 1$ has a maximum $\frac{1}{4}e^{-1} = 0.092$ for $\beta = 1$ and tends to zero in the limit $\beta \to \infty$, whereas the staggered susceptibility χ_x^s increases monotonically as a function of β.

The transverse susceptibility χ_y has a maximum 0.30 for $\beta = 2.40$ and tends to $\frac{1}{4}$ in the limit $\beta \to \infty$.

In figs. 1, 2 and 3 we have drawn the coefficients $a_1(\beta,J)$, $a_2(\beta,J)$ and $a_3(\beta,J)$ as a function of β, for $J = 1$.

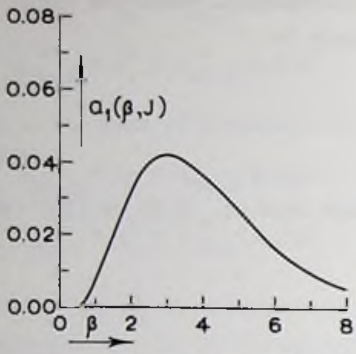

Fig. 1. The coefficient $a_1(\beta,J)$ for J=1, vs. the inverse temperature β.

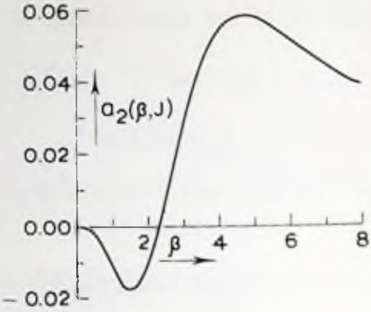

Fig. 2. The coefficient $a_2(\beta,J)$ for J=1, vs. the inverse temperature β.

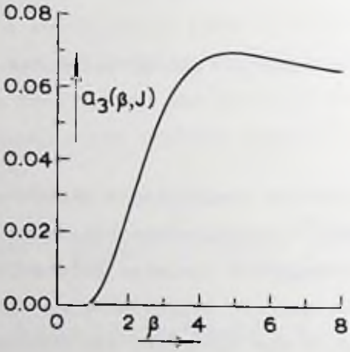

Fig. 3. The coefficient $a_3(\beta,J)$ for J=1, vs. the inverse temperature β.

The coefficient $a_1(\beta,1)$ is negative for high temperatures $0 < \beta < 0.55$ with a minimum -0.00048 for $\beta = 0.38$. For lower temperatures $a_1(\beta,1)$ is positive, reaches a maximum 0.042 for $\beta = 3.04$ and tends to zero in the limit $\beta \to \infty$.

$a_2(\beta,1)$ is negative for $\beta < 2.29$ and positve for $\beta > 2.29$. The coefficient has again two extrema, a minimum -0.017 for $\beta = 1.50$ and a maximum 0.059 for $\beta = 4.69$. For $\beta \to \infty$, $a_2(\beta,1)$ tends to the value $\frac{1}{32}$.

The coefficient $a_3(\beta,1)$ has qualitatively the same features. $a_3(\beta,1)$ is negative for high temperatures $\beta < 0.90$, having a minimum -0.00086 for $\beta = 0.63$. For lower temperatures the coefficient has a maximum 0.070 for $\beta = 4.96$ and tends to $\frac{1}{16}$ in the limit $\beta \to \infty$.

So in the high temperature region the susceptibilities $\chi_{\alpha\alpha,x}$ and $\chi_{\alpha\alpha,z}$ decrease as a function of the applied magnetic field b. For sufficiently low temperatures they all have a mimimum for $b = 0$ and hence must assume a maximum at some finite value of the applied magnetic field. The temperature at which the maximum for $b = 0$ changes into a minimum depends rather strongly on the orientation of the applied field and the element of the susceptibility tensor. In fact, in the case of an Ising chain we have three different temperatures at which this effect can occur, namely the zeros $\beta = 0.55$, $\beta = 2.29$ and $\beta = 0.90$ of the three coefficients $a_1(\beta,1)$, $a_2(\beta,1)$ and $a_3(\beta,1)$.

For the isotropic Heisenberg chain, the antiferromagnetic susceptibility as a function of b has been calculated by Bonner and Fisher [18)]. In the high-temperature region χ has a maximum for $b = 0$, whereas for sufficiently low temperatures χ seems to have a minimum. It is clear that if we change the interaction parameters from values $J_x = J$, $J_y = J_z = 0$ corresponding to the Ising chain, to values $J_x = J_y = J_z = J$ corresponding to the isotropic Heisenberg model, the zeros of $a_1(\beta,1)$, $a_2(\beta,1)$ and $a_3(\beta,1)$ should tend to the same value. This implies in particular that the variation of the zeros is rather large and that the position of the zeros depends rather drastically on the anisotropy of the exchange parameters. Hence by measuring the position of the zeros of the b^2 coefficients of the elements of the susceptibility tensor for various orientations of the magnetic field, one could obtain useful information on the anisotropy of the one-dimensional chain. In connection with this it would be useful to perform finite chain calculations for the elements of the susceptibility tensor for anisotropic Heisenberg chains.

A global impression of the position of the zeros of $a_3(\beta,1)$ may be obtained from the high-temperature expansion up to the order β^6 for the χ_{xx} susceptibility of the anisotropic XY model given in ref. 9 . For the values $\gamma = 1.0$, 0.9, 0.8 and 0.7 of the anisotropy parameter, the zero of the coefficient $a_3(\beta,1)$ occurs at $\beta = 0.84$, 0.89, 0.96 and 1.05 respectively. Obviously the high-temperature expansion is not exact, cf. the values $\beta = 0.84$ and 0.90, but one may conclude that the zero of $a_3(\beta,1)$ will shift to lower temperatures, if the anisotropy decreases from the value $\gamma = 1$

corresponding to the Ising chain, to lower values.

In fig. 4 we have given the coefficients $a_1^s(\beta,J)$, $a_2^s(\beta,J)$ and $a_3^s(\beta,J)$ as a function of β, for $J = 1$.

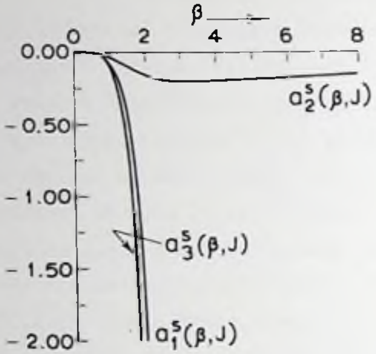

Fig. 4. The coefficients $a_1^s(\beta,J)$, $a_2^s(\beta,J)$ and $a_3^s(\beta,J)$ for J=1, vs. the inverse temperature β.

In contrast to the "non-staggered" quantities $a_\nu(\beta,1)$, all coefficients in fig. 4 are negative for all temperatures. This implies that the staggered susceptibilities $\chi^s_{xx,x}$, $\chi^s_{zz,z}$ and $\chi^s_{xx,z}$ have a maximum for $b = 0$, whereas the other staggered susceptibilities $\chi^s_{yy,x}$, $\chi^s_{zz,x}$ and $\chi^s_{yy,z}$ are equal to "non-staggered" susceptibilities and have a minimum for $b = 0$ for sufficient sufficiently low temperatures.

In fig. 4 the coefficient $a_2^s(\beta,1)$ has a minimum -0.22 for $\beta = 3.29$ and tends to the value $-\frac{5}{32}$ in the limit $\beta \to \infty$; the other two coefficients $a_1^s(\beta,1)$ and $a_3^s(\beta,1)$ decrease monotonically with β.

So far we have discussed the behaviour of the susceptibilities for small values of the applied magnetic field b. We conclude this section, giving the leading term of the asymptotic approximation in the case of a very large applied magnetic field.

For a parallel field $\vec{b} = b\vec{e}_x$, we have, cf. eqs. (2.8), (2.9), (2.22) and (2.24) - (2.27),

$$\chi_{xx,x} \sim \chi^s_{xx,x} = \beta e^{-\beta(b-2J)} + \text{higher exponential terms}, \tag{5.10}$$

$$\chi_{yy,x} = \chi^s_{yy,x} = \chi_{zz,x} = \chi^s_{zz,x} \sim \frac{1}{2(b-2J)} + \text{exponential terms}.$$

In the case of a perpendicular field $\vec{b} = b\vec{e}_z$, the susceptibilities are given by, cf. eqs. (3.6), (3.7), (3.19), (4.29) and (4.30)

$$\chi_{xx,z} = \frac{\tanh \frac{1}{2}\beta b}{2b} - \frac{J}{b^2}(\tanh \tfrac{1}{2}\beta b)^2 + \mathcal{O}\left(\frac{J^2}{b^3}\right),$$

$$\chi^s_{xx,z} = \frac{\tanh \frac{1}{2}\beta b}{2b} + \frac{J}{b^2}(\tanh \tfrac{1}{2}\beta b)^2 + \mathcal{O}\left(\frac{J^2}{b^3}\right),$$

$$\chi_{yy,z} = \chi^s_{yy,z} = \frac{\tanh \frac{1}{2}\beta b}{2b} + \mathcal{O}\left(\frac{J^2}{b^3}\right),$$

$$\chi_{zz,z} = \frac{1}{4}\frac{J^2}{b^3} + \mathcal{O}\left(\frac{J^4}{b^5}\right) + \text{exponential terms},$$

$$\chi^s_{zz,z} = \frac{1}{16}\frac{J^4}{b^5} + \mathcal{O}\left(\frac{J^6}{b^7}\right) + \text{exponential terms}, \tag{5.11}$$

where $\mathcal{O}\left(\frac{J^{2n}}{b^{2n+1}}\right)$ is a shorthand notation for a term proportional to $J^{2n}b^{-(2n+1)}$, whereas the exponential terms contain a factor $e^{-\beta b}$.

6. Interchain interaction

Usually one-dimensional systems can be characterized by a large intrachain coupling and a much smaller interchain coupling between atoms belonging to different chains. For low temperatures the interchain coupling can give rise to long-range magnetic ordering. In the presence of a magnetic field a phase transition can occur at which the long range ordering disappears. Since in general no rigorous treatment can be given for such a phase transition, it seems reasonable to treat the intrachain interactions as exactly as possible and to use an approximate method such as e.g. the molecular field approximation for the interchain interaction. In ref. 20 the magnetic ordering of an Ising chain with interchain interactions was studied along these lines, in the absence of a magnetic field.

Instead of using a molecular field approximation one can also consider a hamiltonian consisting of a relatively large Ising intrachain interaction and a much smaller interaction of the separable or equivalent neighbour type. Such interactions can be treated rigorously in many cases and lead to a free energy per particle which is of the molecular field type [28),29)].

In this section we discuss a system described by the hamiltonian

$$\mathcal{H} = 2J \sum_{\langle i,j \rangle} S_i^x S_j^x - b \sum_i S_i^\gamma + \frac{2J'}{\mathcal{N}} \sum_{\substack{i \in A \\ j \in B}} S_i^\alpha S_j^\alpha \quad , \qquad (6.1)$$
$$(\alpha = x,y,z; \ \gamma = x,y,z) .$$

In this equation it is assumed that the lattice can be divided into two sublattices A and B so that each nearest neighbour of an atom A belongs to sublattice B and vice versa. In the first term of (6.1) we have a summation over all pairs $\langle i,j \rangle$ of nearest neighbours within each of the chains. The last term in (6.1) is an interaction of the equivalent neighbour type between the α components of spins belonging to sublattice A and the α components of spins belonging to sublattice B. Here $\mathcal{N}$ is the total number of atoms in the lattice, i.e. $\mathcal{N} = N \mathfrak{a}$, where $\mathfrak{a}$ is the number of chains and N the number of atoms belonging to a chain. The interaction constant J' can be positive (antiferromagnetic case) as well as negative (ferromagnetic case). Furthermore the second term of (6.1) contains an applied magnetic field which can be parallel ($\gamma = \alpha$) to the exchange coupling J' as well as perpendicular to this coupling ($\gamma \neq \alpha$).

In this section we shall investigate the hamiltonian (6.1) for arbitrary α and γ from a global point of view assuming that the phase transition in an applied magnetic field from long-range magnetic ordering to paramagnetism is of second order. On the basis of this assumption we shall express the critical field in terms of the susceptibilities of the linear chain. Of course the possibility of first-order transitions from long-range ordering to paramagnetism should not be excluded. An investigation of the occurrence of a first-order transition however, would require a much more detailed analysis of the systems under consideration, which is beyond the scope of the present paper. In connection with this we should mention the work by Nagle and Bonner [21),22)], in which an Ising system similar to the hamiltonian (6.1) with $\gamma = x$, $\alpha = x$ has been studied extensively, also in the presence of a finite staggered magnetic field in the x-direction. This system shows many interesting features such as first-order transitions and higher order critical points, especially if the interaction constants J and J' have different signs signs.

Excluding for the moment the special case $\gamma = \alpha$, $J' > 0$ which requires a special treatment, it can be shown that in the thermodynamic limit, the free energy par particle is given by

$$f = \min_{\xi} f[\mathcal{H}_0(\xi)] \tag{6.2}$$

cf. eq. (1.4), where the trial hamiltonian of the linear chain $\mathcal{H}_0(\xi)$ is defined by

$$\mathcal{H}_0(\xi) = T - \xi|J'|\mathcal{M}^\alpha + \tfrac{1}{2}N|J'|\xi^2 \tag{6.3}$$

where

$$T = 2J \sum_i S_i^x S_{i+1}^x - b \sum_i S_i^y \quad . \tag{6.4}$$

The operator $\mathcal{M}^\alpha$ is the magnetization in the ferromagnetic case and the staggered magnetization in the antiferromagnetic case, i.e.

$$\mathcal{M}^\alpha = \sum_{i\in A}{}' S_i^\alpha - J'|J'|^{-1} \sum_{i\in B}{}' S_i^\alpha \tag{6.5}$$

where the primes indicate that the summation over the atoms of sublattices A and B is restricted to the atoms of one chain, so that the summations $i \in A$, $i \in B$ correspond to the summations over even and odd values of i respectively.

Eq. (6.2) can be derived on the basis of the general treatment of the free energy of systems with separable interactions given in ref. 29. For some details we refer to appendix C of the present paper.

The parameter ξ which minimizes the right-hand side of eq. (6.2) must be solved from the molecular field equation

$$\frac{\partial f}{\partial \xi} = 0 \tag{6.6}$$

or equivalently from

$$\xi = N^{-1} \langle e^{-\beta\mathcal{H}_0(\xi)} \mathcal{M}^\alpha \rangle \langle e^{-\beta\mathcal{H}_0(\xi)} \rangle^{-1} \quad . \tag{6.7}$$

If eq. (6.6) has more than one solution, one should select the solution which leads to the lowest value of f.

We now assume that the long-range magnetic ordering is described in terms of a nonvanishing parameter ξ, which tends to zero at the second order transition from long-range ordering to paramagnetism. The critical field can then be obtained from (6.7), considering the solutions with $\xi \neq 0$ in the limit $\xi \to 0$. Clearly, $\xi = 0$ is a solution of (6.7), if we exclude the case $\gamma = \alpha$, $J' < 0$. (In this special case the exchange coupling is ferromagnetic and parallel to the applied field and we would not expect a second order transition.)

For small values of ξ, the right-hand side of (6.7) can be evaluated by perturbation calculation. The result is

$$1 = |J'|N^{-1}\langle e^{-\beta T}\int_0^\beta d\tau\, \mathcal{M}^\alpha \mathcal{M}^\alpha(\tau)\rangle \langle e^{-\beta T}\rangle^{-1}, \quad \gamma \neq \alpha \qquad (6.8)$$

where

$$\mathcal{M}^\alpha(\tau) = e^{\tau T}\mathcal{M}^\alpha e^{-\tau T} \quad , \qquad (6.9)$$

or equivalently

$$|J'|\chi_{\alpha\alpha,\gamma}(b) = 1 \ , \qquad \text{if } J' < 0, \ \ \gamma \neq \alpha \qquad (6.10)$$

$$|J'|\chi^{s}_{\alpha\alpha,\gamma}(b) = 1 \ , \qquad \text{if } J' > 0, \ \ \gamma \neq \alpha. \qquad (6.11)$$

So far we did not consider the case of an antiferromagnetic coupling parallel to the applied field, i.e. $\gamma = \alpha$, $J' > 0$. Since eq. (6.2) is not valid in this case a special treatment is required. This is discussed in some detail at the end of appendix C. As a result, the condition for the occurrence of a second order transition can be written

$$|J'|\chi^{s}_{\alpha\alpha,\alpha}(b - |J'|\eta_0(b)) = 1 \quad , \ J' > 0, \ \ \gamma = \alpha \ , \qquad (6.12)$$

where $\eta_0(b)$ is the α component of the magnetization per particle of the linear chain in the presence of a magnetic field $-(b - |J'|\eta_0(b))$ in the α direction, cf. eq. (C.12).

So far we expressed the phase boundary of a second-order transition from long-range ordering to paramagnetism in terms of a simple relation for the susceptibility of a one-dimensional chain. We shall now discuss to what extent our results can support the qualitative behaviour of the phase boundary separating long-rang magnetic ordering from paramagnetism in cupric sulphate measured by van Tol and Poulis [30),31)]. On this curve the critical temperature as a function of the applied magnetic field b shows a maximum T_{max} for a finite value of b. In particular at temperatures slightly above the Néel temperature T_N two critical fields b_1 and b_2 would occur, the system being paramagnetic for $b < b_1$ and $b > b_2$, whereas for intermediate fields there is long-range ordering. In order to explain this, van Tol and Poulis considered an isotropic antiferromagnetic Heisenberg chain consisting of N spins. The energy levels of such a finite chain have been given by

Bonner and Fisher [18]. Taking into account the lowest two energy levels and extrapolating the results to $N \rightarrow \infty$, van Tol and Poulis were able to obtain a phase boundary curve, having a $T_{max} > T_N$. One should realize however that their treatment does not lead to consistent thermodynamic results, e.g. the entropy of a system of $\mathcal{N}$ spins would be proportional to $\mathcal{N}^{2/3}$, clearly because of the neglect of the higher energy levels of the linear chain. Therefore it seems to be worthwhile to look for an explanation of the effect on the basis of a more rigorous model of a one-dimensional system.

Let us assume for simplicity that the one-dimensional system can be described in terms of an antiferromagnetic Ising interaction. We also assume that the phase transition to the paramagnetic state is a second-order transition as has been observed experimentally [30],[31]*). Then, in view of eqs. (6.10) - (6.12), the phase boundary curve can be described in terms of the susceptibilities discussed in section 5. For sufficiently low temperatures, the susceptibilities described by $a_1(\beta,J)$, $a_2(\beta,J)$ and $a_3(\beta,J)$, i.e. $\chi_{\alpha\alpha,x}$, $\chi_{\alpha\alpha,z}$ $(\alpha = x,y,z)$, $\chi^s_{yy,x} = \chi^s_{zz,x}$ and $\chi^s_{yy,z}$ have a minimum for $b = 0$, so that a maximum should occur for some finite value of b. This implies that at a certain temperature β, eqs. (6.10) - (6.12) can have two different solutions at different values of the applied field for suitable values of the exchange coupling $|J'|$. This could explain, at least in principle, the phase boundary mentioned above.

Unfortunately however, the numerical values of the susceptibilities of an antiferromagnetic chain for small values of b are rather small so that eqs. (6.10) - (6.12) cannot be satisfied, unless the interaction parameter $|J'|$ is much larger than the intrachain coupling J. Under such conditions, the hamiltonian (6.1) does not give a realistic description for a system with short-range interactions. The other susceptibilities $\chi^s_{xx,x}$, $\chi^s_{zz,z}$ and $\chi^s_{xx,z}$, i.e. those described by the coefficients $a^s_1(\beta,J)$, $a^s_2(\beta,J)$ and $a^s_3(\beta,J)$ with the exception of $\chi^s_{zz,z}$ can have large values at low temperatures, but all three susceptibilities have a maximum at $b = 0$ for all temperatures, so that they cannot give an explanation (the presence of the term η_0 in eq. (6.12) does not change this argument).

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*) See also ref. 36 for more recent results.

APPENDIX A

In this appendix we prove eq. (3.8). Using the KMS-property and the operator identity

$$\frac{\partial}{\partial\lambda_j} e^{-\beta\mathcal{H}} = e^{-\beta\mathcal{H}} \int_0^\beta d\tau\; e^{\tau\mathcal{H}}\mathcal{H}_j\; e^{-\tau\mathcal{H}} \tag{A.1}$$

for an arbitrary operator

$$\mathcal{H} \equiv - \sum_j \lambda_j \mathcal{H}_j \tag{A.2}$$

it follows that

$$\int_0^\beta d\tau \;\langle \rho_z S_1^y(\tau) S_{p+1}^y \rangle =$$

$$= \lim_{\substack{b_{y_1}\to 0\\ b_{y_{p+1}}\to 0}} \beta^{-1} Z^{-1} \frac{\partial^2 Z}{\partial b_{y_1}\partial b_{y_{p+1}}} \quad , \tag{A.3}$$

where

$$Z = \langle \exp\left[-\beta(\mathcal{H}_I - b_z \sum_i S_i^z - b_{y_1} S_1^y - b_{y_{p+1}} S_{p+1}^y)\right] \rangle \quad . \tag{A.4}$$

We now evaluate Z using a high-temperature expansion, i.e.

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle \left[\mathcal{H}_I - b_z \sum_i S_i^z - b_{y_1} S_1^y - b_{y_{p+1}} S_{p+1}^y\right]^n \rangle \quad . \tag{A.5}$$

The only terms of (A.5) which can give a nonvanishing contribution to the right-hand side of eq. (A.3) in the limit $b_{y_1} \to 0$, $b_{y_{p+1}} \to 0$ are the terms which are proportional to $b_{y_1} b_{y_{p+1}}$. For $p \neq 0$ such a term is linear in the operator S_1^y and can be written $C\, S_1^y\, D$, where C and D do not contain the operator S_1^y. In order to have a nonvanishing trace, C or D should be linear in the operator S_1^z. Let us suppose that the operator C contains S_1^z, then $C\, S_1^y\, D = L\, S_1^z\, M\, S_1^y\, D$, where the operators L, M and D do not contain the operators S_1^y and S_1^z. Evaluating the right-hand side of eq. (A.5) we also obtain a term L S_1^y M S_1^z D with exactly the same coefficient as the term L S_1^z M S_1^y D. Now the contributions from both terms cancel, since S_1^y M S_1^z = - S_1^z M S_1^y, as is obvious from the relations $S_1^y S_1^z = -S_1^z S_1^y$ and $S_1^y S_1^x S_1^z = - S_1^y S_1^z S_1^x = -S_1^z S_1^x S_1^y$. Hence on the basis of a high-temperature expansion, we have proved that the left-hand side of (A.3) vanishes for $p \neq 0$, which is equivalent to eq. (3.8).

Suppose that eq. (3.8) is not correct for some finite value of the temperature. Then, if the high-temperature expansion would have a finite radius of convergence, the correlation functions would show a nonanalytic behaviour which would correspond to the occurrence of a phase transition. Excluding the possibility of a phase transition in a one-dimensional system with short-range interactions and assuming a finite radius of convergence, we see that eq. (3.8) should be valid at all nonzero temperatures.

APPENDIX B

In this appendix we list the correlation functions and the integrals occurring in eq. (4.10). The correlation functions are given by

$$\begin{aligned}&\langle \rho_I S_{k-1}^x S_{k+1}^x S_1^x S_{p+1}^x \rangle - \\ &- \langle \rho_I S_{k-1}^x S_{k+1}^x \rangle \langle \rho_I S_1^x S_{p+1}^x \rangle = \begin{cases} \frac{1}{16}(-T)^p(1-T^2)(1-\delta_{po}), & \text{if } k=1,\ p+1 \\ \frac{1}{16}(-T)^{p-2}(1-T^4)(1-\delta_{po}), & \text{if } 2 \leq k \leq p \\ 0 & \text{, if } k \geq p+2, \end{cases}\end{aligned} \tag{B.1}$$

$$\begin{aligned}&\langle \rho_I S_k^x S_{k+1}^x S_1^x S_{p+1}^x \rangle - \\ &- \langle \rho_I S_k^x S_{k+1}^x \rangle \langle \rho_I S_1^x S_{p+1}^x \rangle = \begin{cases} \frac{1}{16}(-T)^{p-1}(1-T^2)(1-\delta_{po}), & \text{if } 1 \leq k \leq p \\ 0 & \text{, if } k \geq p+1. \end{cases}\end{aligned} \tag{B.2}$$

Clearly (B.1) and (B.2) vanish for p=0. Furthermore we have

$$\begin{aligned}&\langle \rho_I S_1^x S_{p+1}^x \rangle = \tfrac{1}{4}(-T)^p, \quad \langle \rho_I S_2^x S_{p+1}^x \rangle = \tfrac{1}{4}(-T)^{|p-1|}, \quad \langle \rho_I S_N^x S_{p+1}^x \rangle = \tfrac{1}{4}(-T)^{p+1}, \\ &\langle \rho_I S_N^x S_1^x S_2^x S_{p+1}^x \rangle = \tfrac{1}{16}\left[T^2\delta_{po} + (-T)^p(1-\delta_{po})\right] .\end{aligned} \tag{B.3}$$

The integrals in (4.10) are given by

$$(I_1+I_2+I_3)\sinh^2 J(\tau_1-\tau_2) = \tfrac{1}{4}[-\beta^2 + J^{-2}\sinh^2\beta J] ,$$

$$(I_1+I_2+I_3)\sinh 2J(\tau_1-\tau_2) = \tfrac{1}{4}[-2\beta J^{-1} + J^{-2}\sinh 2\beta J] \tag{B.4}$$

and

$$I_3 \cosh^2 J(\tau_1-\tau_2) = \tfrac{1}{8}[4(\beta-\tau)\tau + 2J^{-2}\cosh^2\beta J - J^{-2}\cosh(2\beta-2\tau)J - J^{-2}\cosh 2\tau J],$$

$$I_3 \sinh^2 J(\tau_1-\tau_2) = \tfrac{1}{8}[-4(\beta-\tau)\tau + 2J^{-2}\cosh^2\beta J - J^{-2}\cosh(2\beta-2\tau)J - J^{-2}\cosh 2\tau J],$$

$$I_3 \sinh 2J(\tau_1-\tau_2) = \tfrac{1}{4}J^{-2}[\sinh 2\beta J - \sinh(2\beta-2\tau)J - \sinh 2\tau J] . \tag{B.5}$$

APPENDIX C

In this appendix we prove eqs. (6.2) - (6.4), following the line of reasoning of ref. 29, section 7. The hamiltonian (6.1) can be written

$$\mathcal{H} = T - \tfrac{1}{2}\mathcal{N}^{-1}|J'|V^2 + \tfrac{1}{2}\mathcal{N}^{-1}|J'|W^2 , \tag{C.1}$$

where

$$T = 2J \sum_{(i,j)} S_i^x S_j^x - b \sum_i S_i^y , \tag{C.2}$$

$$V = [\sum_{i\in A} S_i^\alpha - J'|J'|^{-1} \sum_{i\in B} S_i^\alpha], \tag{C.3}$$

$$W = [\sum_{i\in A} S_i^\alpha + J'|J'|^{-1} \sum_{i\in B} S_i^\alpha]. \tag{C.4}$$

According to ref. 29, the free energy per particle is given by

$$f = \min_{\xi} \max_{\eta} f[\tilde{\mathcal{H}}_0(\xi,\eta)] , \tag{C.5}$$

where

$$\tilde{\mathcal{H}}_0(\xi,\eta) = T - |J'|\xi V + |J'|\eta W + \tfrac{1}{2}\mathcal{N}|J'|(\xi^2-\eta^2) . \tag{C.6}$$

Eq. (C.5) is correct, since

$$\lim_{\mathcal{N}\to\infty} \mathcal{N}^{-2}\left\langle \frac{\exp[-\beta\tilde{\mathcal{H}}_0(\xi,\eta)]}{\langle \exp[-\beta\tilde{\mathcal{H}}_0(\xi,\eta)]\rangle} \left(W - \frac{\langle \exp[-\beta\tilde{\mathcal{H}}_0(\xi,\eta)]W\rangle}{\langle \exp[-\beta\tilde{\mathcal{H}}_0(\xi,\eta)]\rangle}\right)^2\right\rangle = 0. \tag{C.7}$$

Eq. (C.7) follows from the fact that the hamiltonian $\tilde{\mathcal{H}}_0(\xi,\eta)$ is a linear combination of independent hamiltonians of linear chains, so that the average at the left-hand side of (C.7) can be factorized as a product of averages over linear chains. As a result the average at the left-hand side of (C.7) can be written as $\mathcal{A}^{-1}N^{-2}\Sigma_{i,j}C_{ij}$, where $\mathcal{A}$ is the number of chains, N the number of atoms in a chain and C_{ij} are intrachain correlation functions. In the thermodynamic limit $\mathcal{A}$ tends to infinity and the left-hand side of (C.7) vanishes.

Since $\tilde{\mathcal{H}}_0(\xi,\eta)$ is a linear combination of hamiltonians of independent linear chains, the free energy can also be expressed in terms of the free energy per particle of one linear chain. We have

$$f = \min_{\xi} \max_{\eta} f[\mathcal{H}_0(\xi,\eta)] \,, \tag{C.8}$$

where

$$\mathcal{H}_0(\xi,\eta) = T - |J'|(\xi-\eta)\sum_{i\in A}{}' S_i^\alpha + J'(\xi+\eta)\sum_{i\in B}{}' S_i^\alpha + \tfrac{1}{2}N|J'|(\xi^2-\eta^2). \tag{C.9}$$

Here ξ and η are the solutions of the molecular field equations

$$\frac{\partial f}{\partial \xi} = 0, \qquad \frac{\partial f}{\partial \eta} = 0 \,, \tag{C.10}$$

which lead to the lowest value of f. Eqs. (C.10) can also be written

$$\xi = \frac{1}{N}\left\langle e^{-\beta\mathcal{H}_0(\xi,\eta)}\left[\sum_{i\in A}{}' S_i^\alpha - J'|J'|^{-1}\sum_{i\in B}{}' S_i^\alpha\right]\right\rangle \left\langle e^{-\beta\mathcal{H}_0(\xi,\eta)}\right\rangle^{-1}, \tag{C.11}$$

$$\eta = \frac{1}{N}\left\langle e^{-\beta\mathcal{H}_0(\xi,\eta)}\left[\sum_{i\in A}{}' S_i^\alpha + J'|J'|^{-1}\sum_{i\in B}{}' S_i^\alpha\right]\right\rangle \left\langle e^{-\beta\mathcal{H}_0(\xi,\eta)}\right\rangle^{-1}. \tag{C.12}$$

Eq. (C.12) has a solution $\eta = 0$, unless $\gamma = \alpha$ and $J' > 0$. This is obvious in the ferromagnetic case with $J' < 0$, since the hamiltonian $\mathcal{H}_0(\xi, 0)$ is invariant under a translation over one lattice distance in the linear chain, so that the average values of the α components of the spins belonging to the sublattices A and B are equal. In the antiferromagnetic case with $\gamma \neq \alpha$, the hamiltonian $\mathcal{H}_0(\xi,0)$ is invariant under a rotation over π around the γ axis, followed by a translation over one lattice distance. This implies that the average value of the α component of a spin of sublattice A is minus the average value of the α component of a spin of sublattice B. In both cases we see that eq. (C.12) has a solution $\eta = 0$. Since according to ref. 29, the second molecular field equation $\partial f/\partial\eta = 0$ defines a unique function

$\eta \equiv \eta(\xi)$, $\eta = 0$ is the only solution of eq. (C.12). Now esq. (6.2) - (6.4) are obvious, unless $\gamma = \alpha$ and $J' > 0$, after inserting $\eta = 0$ in eq. (C.9) and (C.11).

We finally discuss the special case that $\gamma = \alpha$ and $J' > 0$. Clearly eq. (C.12) has a solution $\eta_0(b) \neq 0$ for $\xi = 0$ in the presence of the magnetic field $b\vec{e}_\alpha \equiv b\vec{e}_\gamma$. Then, expanding (C.12) for small values of the parameters ξ and $\Delta\eta \equiv \eta - \eta_0$, one finds

$$\Delta\eta = -|J'|\chi_{\alpha\alpha,\alpha}\Delta\eta + \text{quadratic terms.} \tag{C.13}$$

In particular, the linear term in ξ vanishes and each solution $\Delta\eta \neq 0$ must be quadratic in ξ. This implies that we can neglect the terms with $\Delta\eta$, if we are interested in the linear terms in ξ in eq. (C.11). For small values of ξ, eq. (C.11) reduces to

$$\xi = |J'|\xi \int_0^\beta d\tau \, \langle e^{-\beta\tilde{T}} \mathcal{M}^\alpha \mathcal{M}^\alpha(\tau) \rangle \, \langle e^{-\beta\tilde{T}} \rangle^{-1} \tag{C.14}$$

where

$$\mathcal{M}^\alpha(\tau) = e^{\tau\tilde{T}} \mathcal{M}^\alpha e^{-\tau\tilde{T}} \tag{C.15}$$

and

$$\tilde{T} = 2J \sum_i S_i^x S_{i+1}^x - [b - |J'|\eta_0(b)] \sum_i S_i^\alpha - \tfrac{1}{2}N|J'|\eta_0^2(b) \, . \tag{C.16}$$

Now eq. (6.12) is obvious from (C.14).

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SAMENVATTING

Een belangrijk probleem in de statistische mechanica is de berekening van thermodynamische grootheden voor een veel-deeltjes systeem, uitgaande van de microscopische wisselwerkingen tussen de deeltjes. Hiertoe moet men de logaritme van de toestandssom (of de vrije energie) per deeltje bepalen. Door differentiëren kunnen dan de thermodynamische grootheden van het systeem worden afgeleid. In veel gevallen is een exacte berekening niet mogelijk. In verband hiermee kan het van belang zijn eenvoudige modelsystemen te bestuderen. In dit proefschrift wordt aandacht besteed aan enige aspecten van één-dimensionale quantum spin systemen (spin $\frac{1}{2}$) met anisotrope exchange wisselwerkingen tussen naaste buren onder invloed van een uitwendig magneetveld. De resultaten kunnen ook experimenteel van belang zijn in het geval van (drie-dimensionale) systemen, die bestaan uit een aantal ketens, zodanig, dat de wisselwerking binnen de ketens veel sterker is dan die tussen de ketens.

In hoofdstuk I van dit proefschrift wordt een hoge temperatuur ontwikkeling gegeven tot en met β^6, $(\beta = (kT)^{-1})$, voor het xx element χ_{xx} van de susceptibiliteitstensor van het één-dimensionale XY model. Bij de berekening wordt gebruik gemaakt van een projectie operator methode, die het mogelijk maakt gemiddelden van operatoren in het spin-cyclische XY model uit te drukken in gemiddelden over het c-cyclische en het c-anticyclische XY model. Hierbij moet voor χ_{xx} een gemiddelde worden berekend van produkten van operatoren, waarin een factor voorkomt die zowel de c-cyclische als de c-anticyclische hamiltoniaan bevat. Deze factor, die niet optreedt bij de berekening van χ_{zz}, maakt een exacte berekening van χ_{xx} onmogelijk. Tevens wordt aangetoond dat de χ_{xx}-susceptibiliteit per deeltje in het spin-cyclische model verschilt van die in het c-cyclische model, zelfs in de thermodynamische limiet. Dit illustreert de moeilijkheden, die kunnen optreden, wanneer het c-cyclische model gebruikt wordt voor de berekening van thermodynamische grootheden.

In hoofdstuk II wordt het anisotrope één-dimensionale Heisenberg model met verschillende exchange constanten J_x, J_y en J_z beschouwd. Gebruikmakend van een eerste orde storingsrekening in J_z en tevens van eerder gevonden resultaten voor het anisotrope XY model en een hoge temperatuurontwikkeling voor het isotrope geval met $J_x = J_y = J_z$, wordt een hoge temperatuurontwikkeling gegeven voor de soortelijke warmte per deeltje tot en met orde β^9 en voor χ_{zz} tot en met orde β^6 .

In hoofdstuk III worden resultaten gegeven,die ook geldig zijn voor lage temperaturen. De elementen van de susceptibiliteitstensor van een Ising keten in een parallel en loodrecht magneetveld worden exact berekend,behalve de parallel susceptibiliteit χ_{xx} in een loodrecht veld (Deze wordt met behulp van storingsrekening behandeld). Voor voldoend lage temperaturen vertoont de susceptibiliteit van een antiferromagnetische Ising keten een minimum voor $b = 0$ en bijgevolg een maximum voor een eindig magneetveld b. Ook worden de staggered susceptibiliteiten gegeven. Tenslotte wordt een discussie gegeven die betrekking heeft op de overgang van antiferromagnetisme naar paramagnetisme in systemen bestaande uit zwak gekoppelde lineaire ketens.

Studiegegevens:

Na in juni 1966 het eindexamen gymnasium β te hebben afgelegd aan het Dalton Lyceum in Den Haag, begon ik in september van dat jaar sterrenkunde en natuurkunde te studeren aan de Rijksuniversiteit te Leiden.

Het kandidaatsexamen sterrenkunde en natuurkunde met bijvak wiskunde legde ik af in maart 1969 en het doctoraalexamen theoretische natuurkunde met bijvak wiskunde in februari 1972. Het experimentele werk werd verricht in de Metalengroep onder leiding van Dr. G.J. van den Berg.

Gedurende het cursusjaar 1972-1973 gaf ik les in natuurkunde aan de Scholengemeenschap Zandvliet in Den Haag.

Sinds augustus 1973 ben ik als natuurkundeleraar verbonden aan het Stedelijk Gymnasium te Leiden.

In februari 1973 werd een begin gemaakt met het onderzoek dat aan dit proefschrift ten grondslag ligt. Hoofdstuk I en II zijn tot stand gekomen in nauwe samenwerking met Dr. Th.J. Siskens.

Het typewerk werd verzorgd door mevrouw S. Hélant Muller-Soegies. De tekeningen werden vervaardigd door de heer W.J. Tegelaar.

STELLINGEN

behorende bij het proefschrift van

E.J. VAN DONGEN

Leiden
16 juni 1976

1. De bestudering van buigpunten in magnetisatie-isothermen van één-dimensionale (antiferromagnetische) spinsystemen kan inzicht geven in de mate van anisotropie van de wisselwerking tussen de spins.

   Hoofdstuk III van dit proefschrift.

2. Voor een één-dimensionaal Ising model met xx-koppelingen en een magneetveld b in de z-richting zijn de correlatiefuncties $\langle \rho S^y_1(\tau)\, S^y_{p+1} \rangle$ voor $p \geq 2$ tot en met orde b^2 gelijk aan nul.

   Hoofdstuk III van dit proefschrift.

3. Het feit dat Van Hemmen en Vertogen het verschil in uitkomst tussen de transversale susceptibiliteit voor het a-cyclische en c-cyclische XY model als "meer dan verrassend" ervaren, illustreert het belang van een precieze omschrijving van de thermodynamische-limiet-procedure.

   J.L. van Hemmen en G. Vertogen, Physica 81A (1975) 391.
   Hoofdstuk I van dit proefschrift.

4. Bij de microscopische afleiding van de Fokker-Planck-vergelijking maakt Résibois gebruik van een commutatierelatie voor de projectie-operator. Deze relatie is onjuist, maar beïnvloedt het eindresultaat niet.

   P. Résibois, Electrolyte Theory, Harper and Row (New York, Evanston and London, 1968) 68.

5. De verklaring die Reith en Swinney geven voor het verloop van de depolarisatiefactor als functie van het temperatuurverschil $T-T_c$ voor hun lichtverstrooiings-experiment is onjuist.

   L.A. Reith en H.L. Swinney, Phys.Rev. A12 (1975) 1094.

6. De methode die Guertin e.a. gebruiken om legeringen van palladium en zeldzame aarden te homogeniseren is niet toereikend.

   R.P. Guertin, H.C.Praddaude, S. Foner, E.J. McNiff Jr. en B. Barsoumian, Phys.Rev. B7 (1973) 274.

7. De experimentele gegevens over de anomalie in de y-verdeling en de produktie van muonparen bij anti-neutrino-hadron verstrooiing zijn niet in overeenstemming met een gemeenschappelijke verklaring voor beide effecten, zoals gesuggereerd door Benvenuti e.a.

   A. Benvenuti, D. Cline, W.T. Ford, R. Imlay, T.Y. Ling, A.K. Mann, F. Messing, R. Orr, D.D. Reeder, C. Rubbia, R. Stefanski, L. Sulak en P. Wanderer, Phys.Rev.Letters 35 (1975) 1249 en 34 (1975) 597.

8. In een aantal klassieke één-dimensionale spinsystemen met alternerende wisselwerkingen treedt onder invloed van een uitwendig magneetveld voor T=0 slechts één fase-overgang op, in tegenstelling tot het geval van een alternerende quantummechanische XY keten.

   J.H.H. Perk, H.W. Capel, M.J. Zuilhof en Th.J. Siskens, Physica 81A (1975) 319.

9. In het boek "Théorie du Magnétisme" van A. Herpin zal men tevergeefs zoeken naar de numerieke waarden van de half-tallige Brillouin functies.

   A. Herpin, Théorie du Magnétisme, Presses universitaires de France (Paris, 1968) 132, 133.

10. Het gebruik van leesteksten bij het onderwijs in de natuurkunde op het V.W.O. kan een bijdrage leveren tot een beter begrip van de natuurkunde.