nicht die S-Matrix als Funktion der Energie, sondern nur bei fester, durch das Experiment vorgegebener Energie zu berechnen. Lediglich bei Streuproblemen mit großem Coulomb-Parameter η wird die Auswertung durch die zu diagonalisierenden umfangreichen Matrizen erschwert.

Die detaillierte Durchführung der vorgelegten Theorie am Beispiel der Coulomb-Anregung der Rotationsniveaus deformierter Kerne ist in Vorbereitung.

Meinem verehrten Lehrer, Herrn Professor Dr. O. SCHERZER, danke ich für sein Interesse, das er diesem Problem entgegenbrachte und für wertvolle Anregungen und Ratschläge bei der Fertigstellung dieser Arbeit. Die Problemstellung der Arbeit ergab sich aus Diskussionen mit meinem Bruder, Professor Dr. W. GREINER, wofür ich ihm danken möchte. Dank gebührt auch den Herren Dr. C. TOEPFFER, Dr. W. SCHEID und K. SCHÄFER für Diskussionen und Hinweise.

Correlation Function Approach to Short-Range Order in the Ising-Model

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By pushing forward the decoupling from the three- to the four-point correlation function short-range order is systematically introduced into the description of the statistical behaviour of the Ising-model. Application of a procedure which is a natural generalization of that invented by Bogoljubov and Tjablikov for the Heisenberg-model, leads to an overall-approximation for the magnetization and the nearest-neighbour correlation which may be compared with the Ising-model variant of Oguchi's two-spin-cluster molecular field theory. The results of both approximations are very similar both for low and high temperatures, but for the transition point the new approach yields values which lie considerably lower and therefore are more reliable than those following from Oguchi's theory. Moreover, the comparison with a slight modification of the theory which is also presented in this paper, illuminates the physical mechanism which is responsible for the formation of correlations within the order of approximation, considered.

1. Introduction

Beyond any doubt the technique of quantum-statistical Green's functions and correlation functions is one of the most powerful tools in the modern theory of interacting N-particle systems in general and in the theory of magnetism in particular.

Applied to the Heisenberg ferromagnet already its simplest version which consists of a decoupling approximation in the three-point function as given by BOGOLJUBOV and TJABLIKOV [1, 2], leads to a description of the temperature dependence of the magnetization, in which the correct low temperature behaviour of this quantity is incorporated as well as a phase transition. After some slight modifications in the decoupling procedure this approximation yields the best overall-description of the Heisenberg-model existing up to this day.

On the other hand it clearly suffers from the fact of being essentially a single particle theory, in which statistical correlations of the z-components of spins at different lattice sites are neglected in the same way as they are in the Weiss molecular field approximation. Clearly, this is due to the fact that the decoupling is performed in the three-point function. But unfortunately great mathematical difficulties arise, if one tries to push this decoupling forward to a higher order of these functions and thus to take into account correlation effects in spin-clusters as this was done by OGUCHI [3] or P. R. WEISS [4] within the frame of molecular field theories.

For the Ising-model the chain of Green's functions may be explicitly summed up because of the

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simple commutation properties of its Hamiltonian [5, 6], yielding a set of exactly valid equations for thermodynamic averages which unfortunately does not completely determine the problem. On the other hand the introduction of the decoupling of Bogoljubov and Tjablikov (BT) into the three-point function at once leads to the Weiss molecular field approximation (WMF) which by this way proves to be the Ising counterpart of the BT-approximation for the Heisenberg-model. But contrary to this model the Ising-model is simple enough to permit an explicit consideration of correlating effects by the method of correlation functions.

For this purpose certain parts of the three-point functions must be considered in the equations of motion exactly by shifting the decoupling from those to the four-point functions. In this way the molecular field results of Oguchi or their Ising counterpart may be reproduced, when the three-point function of a given cluster consisting of two spins is taken into account explicitly [7, 8].

In this paper we present the results of an alternative decoupling of the four-point functions which in some respect is the natural generalization of the BT procedure, and leads to a description of the phase-transition and the short-range order in the Ising-model which seems not to be discussed in the literature on this subject. This approximation is not claimed for being an especially good one in comparison with the results of the sophisticated methods available for the Ising-model today – see e. g. [9] –, but it seems to provide a better description of the model just in the critical region than the simple two-spin-cluster theory does, though the order of approximation is exactly the same for both approaches.

Moreover, the consideration of a slight modification of the theory presented in this paper illuminates the physical mechanism which brings about correlations within this order of approximation.

2. Approximative Integration of the Equations of Motion

The Ising-model with nearest-neighbour interactions which we are concerned with in this paper, is determined by the Hamiltonian

$$\mathbf{H} = -J \sum_{n,\Delta} \mathbf{s}_n^z \, \mathbf{s}_{n+\Delta}^z , \tag{1 a}$$

where $\boldsymbol{\Delta}$ represents the z nearest-neighbour vectors of the coordination lattice considered and $(\mathbf{s}_n^z)^2 = \frac{1}{4}$ holds; the additional influence of a homogeneous external magnetic field directed along the z-axis is given by

$$\mathbf{H}_z = H' \sum_n \mathbf{s}_n^z \tag{1 b}$$

with H' connected with the gyromagnetic factor g, Bohr's magneton μ_B and the magnetic field H_z by

$$H' = g \, \mu_B \, H_z . \tag{1 c}$$

The method, we shall apply to this model, is simple and closely akin to a procedure which SAUTER [10] has extracted from the more complicated formalism of Green's functions for the application to the Heisenberg-model:

Let us define the correlation functions $\langle \mathbf{s}_m^+, \mathbf{s}_{m+l}^- \rangle$ and $\langle \mathbf{s}_m^+ \mathbf{s}_{m+\Delta}^z, \mathbf{s}_{m+l}^- \rangle$, where the meaning of $\langle \mathbf{A}, \mathbf{B} \rangle$ is

$$\langle \mathbf{A}, \mathbf{B} \rangle = \langle \mathbf{A}(t) \, \mathbf{B}(0) \rangle \tag{2}$$

and $\mathbf{s}_m^{\pm}$ are the spin-deviation operators, defined by

$$\mathbf{s}_m^{\pm} = \mathbf{s}_m^x \pm i \, \mathbf{s}_m^y . \tag{3}$$

By virtue of the translation invariance of the Hamiltonian (1) these functions will not depend on the lattice site $\boldsymbol{m}$, so that we may write

$$\begin{aligned} f_l(t) &= \langle \mathbf{s}_m^+ , \mathbf{s}_{m+l}^- \rangle , \\ h_{l,\Delta}(t) &= \langle \mathbf{s}_m^+ \, \mathbf{s}_{m+\Delta}^z , \mathbf{s}_{m+l}^- \rangle . \end{aligned} \tag{4}$$

We now investigate the equation of motion for the two-point function $f_l(t)$ which is given by

$$\begin{aligned} i \frac{\mathrm{d}}{\mathrm{d}t} f_l(t) &= \langle [\mathbf{s}_m^+, \mathbf{H} + \mathbf{H}_z], \mathbf{s}_{m+l}^- \rangle \\ &= -H' f_l(t) + 2J \sum_{\Delta} h_{l,\Delta}(t) . \end{aligned} \tag{5}$$

The wellknown procedure of BT consists in decoupling $h_{l,\Delta}(t)$ according to

$$h_{l,\Delta}(t) = \langle \mathbf{s}^z \rangle \, f_l(t) = s \, f_l(t) , \tag{6}$$

whereby (5) becomes an equation purely in $f_l(t)$. From its integration one easily gets Weiss' molecular field approximation by use of the thermodynamic boundary conditions – see Eq. (14) later on – for the correlation functions.

[5] B. G. S. DOMAN and D. TER HAAR, Physics Letters **2**, 15 [1962].
[6] H. B. CALLEN, Physics Letters **4**, 161 [1963].
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[9] C. DOMB, Adv. Physics **9**, 149 [1960].
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In this paper we do not perform any decoupling in $h_{l,\Delta}(t)$, but go on to formulate the equation of motion for this function, too. By

$$\left(i\frac{\mathrm{d}}{\mathrm{d}t}+H'\right)h_{l,\Delta}(t)=2J\sum_{\Lambda}\langle \mathbf{s}_m^+\,\mathbf{s}_{m+\Delta}^z\mathbf{s}_{m+\Lambda}^z\,,\,\mathbf{s}_{m+l}^-\rangle \tag{7}$$

this three-point function is connected with four-point functions.

Now it is crucial to note that in one summand on the right hand of Eq. (7) $\mathbf{\Lambda}=\mathbf{\Delta}$ holds, whereby the corresponding four-point function is reduced to $\frac{1}{4}f_l$ because of $(\mathbf{s}^z)^2=\frac{1}{4}$. In fact, as will be shown in Chapter 4, this is the only mechanism that gives rise to two-spin-correlations within the order of approximation we are going to introduce now:

If $\mathbf{\Delta}$ and $\mathbf{\Lambda}$ differ, we get four-point functions, the graph of which is given in Fig. 1. Neglecting

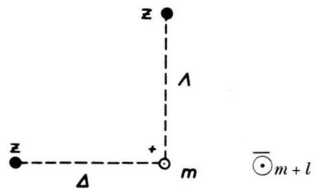

Fig. 1. Graph of the four-point correlation functions.

the correlation of any three spins systematically, we next perform the symmetric decoupling

$$\begin{aligned}&\langle \mathbf{s}_m^+\,\mathbf{s}_{m+\Delta}^z\,\mathbf{s}_{m+\Lambda}^z\,,\,\mathbf{s}_{m+l}^+\rangle\\ &\approx\tfrac{1}{2}s\{\langle \mathbf{s}_m^+\,\mathbf{s}_{m+\Lambda}^z\,,\,\mathbf{s}_{m+l}^-\rangle+\langle \mathbf{s}_m^+\,\mathbf{s}_{m+\Delta}^z\,,\,\mathbf{s}_{m+l}^-\rangle\}\\ &=\tfrac{1}{2}s\{h_{l,\Lambda}(t)+h_{l,\Delta}(t)\}\,.\end{aligned}\tag{8}$$

This procedure should be especially reliable for lattice types, where the sites $\boldsymbol{m}+\mathbf{\Delta}$ and $\boldsymbol{m}+\mathbf{\Lambda}$ may not be nearest neighbours, as is the case for all plane and cubic coordination lattices apart from the triangle and the f. c. c. lattice.

Now introduce (8) into Eq. (7) and define

$$g_l(t)=\sum_{\Delta}h_{l,\Delta}(t)\,. \tag{9}$$

Gathering up the result of this procedure and Eq. (5) we, for one thing, get a system of coupled first order differential equations for the motion of f_l and g_l

$$i\begin{pmatrix}\dot{f}_l\\ \dot{g}_l\end{pmatrix}=\begin{pmatrix}-H' & 2J\\ \frac{1}{2}zJ & -H'+2J(z-1)s\end{pmatrix}\begin{pmatrix}f_l\\ g_l\end{pmatrix} \tag{10 a}$$

and, for another thing, an equation for $h_{l,\Delta}$

$$i\dot{h}_{l,\Delta}+(H'-J(z-2)s)\;h_{l,\Delta}=\frac{J}{2}f_l+Jsg_l \tag{10 b}$$

which depends on this system.

These equations are easily solved. Defining

$$\begin{aligned}\varepsilon_{1,2,3}&=J\eta_{1,2,3}-H',\\ \eta_{1,2}&=s(z-1)\pm\sqrt{s^2(z-1)^2+z}\,,\;\eta_3=s(z-2),\\ E_i&=e^{-i\varepsilon_i t}\end{aligned}\tag{11}$$

for convenience, we get the solutions

$$\begin{pmatrix}f_l(t)\\ g_l(t)\end{pmatrix}=\frac{1}{\eta_1-\eta_2}\begin{pmatrix}-\eta_2E_1+\eta_1E_2 & 2(E_1-E_2)\\ \frac{1}{2}z(E_1-E_2) & \eta_1E_1-\eta_2E_2\end{pmatrix}\begin{pmatrix}f_l(0)\\ g_l(0)\end{pmatrix} \tag{12 a}$$

and

$$h_{l,\Delta}(t)=\frac{1}{z}g_l(t)-\left\{\frac{1}{z}g_l(0)-h_{l,\Delta}(0)\right\}E_3\,. \tag{12 b}$$

With them we have got all information concerning the dynamical features of the model required and may proceed to the investigation of the statistical ones in the next chapter.

3. The Statistical Consequences of the Approximation

The point of contact between dynamics and statistics is given by the famous relation

$$\langle \mathbf{A}(t)\,\mathbf{B}(0)\rangle=\langle \mathbf{B}(0)\,\mathbf{A}(t+i\beta)\rangle \tag{13}$$

holding for the macro-canonical ensemble, from which we get

$$\langle[\mathbf{A},\mathbf{B}]\rangle=\langle \mathbf{A}(0)\,\mathbf{B}(0)\rangle-\langle \mathbf{A}(-i\beta)\,\mathbf{B}(0)\rangle \tag{14}$$

by setting $t=-i\beta$. This equation will be the starting point for our further considerations.

If we define

$$\begin{aligned}F_l&=\langle[\mathbf{s}_m^+\,,\,\mathbf{s}_{m+l}^-]\rangle\,,\\ G_l&=\langle[\mathbf{s}_m^+\sum_{\Delta}\mathbf{s}_{m+\Delta}^z\,,\,\mathbf{s}_{m+l}^-]\rangle\,,\\ H_{l,\Delta}&=\langle[\mathbf{s}_m^+\,\mathbf{s}_{m+\Delta}^z\,,\,\mathbf{s}_{m+l}^-]\rangle\end{aligned}\tag{15}$$

and choose $\boldsymbol{l}=\mathbf{0}$, we can reduce these and the functions $f_0(0)$, $g_0(0)$ and $h_{0,\Delta}(0)$ by virtue of the peculiarities of the spin-1/2-algebra with the result

$$\begin{aligned}&F_0=2s\,, && f_0(0)=\tfrac{1}{2}+s\,,\\ &H_{0,\Delta}=2q(\mathbf{\Delta})=\langle \mathbf{s}_m^z\mathbf{s}_{m+\Delta}^z\rangle\,, && h_{0,\Delta}(0)=\tfrac{1}{2}s+q(\mathbf{\Delta})\,,\\ &G_0=2\sum_{\Delta}q(\mathbf{\Delta})\,, && g_0(0)=\frac{z}{2}s+\sum_{\Delta}q(\mathbf{\Delta})\,.\end{aligned}\tag{16}$$

In consequence of the point-symmetry of the lattice types considered, we may suggest that $q(\mathbf{\Delta})$ will not depend on $\mathbf{\Delta}$ in fact[11]. Hence we may confine our

[11] It is possible to prove this conjecture by a systematic discussion of the complete system of solutions (12 a) and (12 b).

further attention to the behaviour of the function g_0 which is simpler than that one of $h_{0,\Delta}$.

Setting

$$\hat{E}_i = e^{-\beta \varepsilon_i} \tag{17}$$

in analogy to the definition of E_i and combining (14), (16) and (12 a) we get after some re-arrangement

$$\begin{aligned}&\{\eta_1 - \eta_2 - \eta_2 \hat{E}_1 + \eta_1 \hat{E}_2 + z(\hat{E}_1 - \hat{E}_2)\}\, s \\ &\quad + 2\, z(\hat{E}_1 - \hat{E}_2)\, q = \tfrac{1}{2}\{\eta_1 - \eta_2 + \eta_2 \hat{E}_1 - \eta_1 \hat{E}_2\} \\ &\tfrac{1}{2}\{-\eta_1 + \eta_2 + \hat{E}_1 - \hat{E}_2 + \eta_1 \hat{E}_1 - \eta_2 \hat{E}_2\}\, s \\ &+ \{\eta_1 - \eta_2 + \eta_1 \hat{E}_1 - \eta_2 \hat{E}_2\}\, q = -\tfrac{1}{4}(\hat{E}_1 - \hat{E}_2).\end{aligned} \tag{18}$$

By these equations the magnetization s and the (z,z)-correlation q are fully determined.

To improve the transparency of the evaluation of s and q from these equations, it is useful to introduce some abbreviations:

$$\begin{aligned}&\eta_{1,2} = \mu \pm \nu, \\ &\mu = s(z-1),\ \nu = \sqrt{s^2(z-1)^2 + z} = \sqrt{\mu^2 + z}, \\ &A = e^{\beta(H' - J\mu)} = e^{\beta(H' - J\, s(z-1))}, \\ &S = \sinh(\beta J \nu),\ C = \cosh(\beta J \nu).\end{aligned} \tag{19}$$

Using them, after a somewhat tedious elimination we get the relations

$$\nu A^2(s + \tfrac{1}{2}) + A\, s\,(2\nu C - (z+1)\, S) + \nu(s - \tfrac{1}{2}) = 0, \tag{20 a}$$

$$q = \frac{1}{4\, z\, A\, s}\{2[\nu + (\mu - z)\, A S + \nu A C]\, s - [\nu - \mu A S - \nu A C]\}, \tag{20 b}$$

the first of which is an implicit non-linear equation for the determination of $s(T)$, whereas the second one allows the calculation of q, when s is known.

Eq. (20 a) may be brought into a form, in which it is very similiar to that of the two-spin-cluster theory which is derived in Appendix 1.

For both theories we find

$$s = -\frac{\sinh(\beta H_{\text{eff}})}{2\cosh(\beta H_{\text{eff}}) + \Gamma}, \tag{21}$$

but whereas the Oguchi type molecular field approach yields

$$H_{\text{eff}} = H' - 2\, J\, s(z-1),\ \Gamma = 2\, e^{-\beta J}, \tag{22 a}$$

we now get

$$\begin{aligned}&H_{\text{eff}} = H' - J\, s(z-1), \\ &\Gamma = 2\, C - \frac{z+1}{\nu} S \\ &= 2\cosh\left(\beta J \sqrt{s^2(z-1)^2 + z}\right) - \frac{z+1}{\sqrt{s^2(z-1)^2 + z}} \\ &\quad \cdot \sinh\left(\beta J \sqrt{s^2(z-1)^2 + z}\right).\end{aligned} \tag{22 b}$$

For q a comparably simple expression does not seem to exist, but clearly this quantity is uniquely determined by (20 b).

4. A Modification of the Approach of the Last Chapters

Before discussing the quantitative contents and physical consequences of the formulae (20), (21) and (22), we now go to present a slight modification of the derivation given so far, which is interesting by the fact that it sheds a striking light on the mechanism bringing about correlations-effects within the order of approximation considered.

For this purpose let us go back to Eq. (7), but forget the fact that in one of the z summands on the right hand of this equation $\mathbf{\Delta}$ and $\mathbf{\Lambda}$ are identical. Performing the decoupling (8) now and introducing $g_l(t)$ as given by (9), instead of (10 a) we get the equations

$$i\begin{pmatrix}\dot{f}_l \\ \dot{g}_l\end{pmatrix} = \begin{pmatrix}-H' & 2J \\ 0 & -H' + 2\, J\, s\, z\end{pmatrix}\begin{pmatrix}f_l \\ g_l\end{pmatrix} \tag{23}$$

which describe the dynamical aspects of the system in this case.

Integration of these differential equations and application of exactly the same procedure as was performed on the way from (10) to Eqs. (18), yields the relations

$$\begin{aligned}&(s - \tfrac{1}{2}) = -\hat{E}_1'(s + \tfrac{1}{2}) - (\hat{E}_2' - \hat{E}_1')(\tfrac{1}{2} + q/s), \\ &(q - \tfrac{1}{2}\, s) = -\hat{E}_2'(q + \tfrac{1}{2}\, s)\end{aligned} \tag{24}$$

where $\hat{E}_1'$ and $\hat{E}_2'$ are defined by

$$\hat{E}_1' = e^{\beta H'}, \qquad \hat{E}_2' = e^{\beta(H' - 2\, J\, s\, z)} \tag{25}$$

for the sake of simplicity.

Evaluating these equations one finds from the second line of (24)

$$\frac{q}{s} = \frac{1}{2}\left(\frac{1 - \hat{E}_2'}{1 + \hat{E}_2'}\right) \tag{26}$$

and introducing this and (25) into the first equation one finally gets

$$s = \tfrac{1}{2}\tanh[\tfrac{1}{2}\beta(-H' + 2\, J\, s\, z)],\ q = s^2. \tag{27}$$

This is exactly the result of Weiss' (one-spin-cluster) molecular field theory, in which correlations between different particles are neglected from the beginning. It looks pretty surprising to recover these relations, especially $q = s^2$, as the result of a procedure which

was supposed to yield a better description of the model, because the decoupling is performed in a way which takes correlating effects into account. But it clearly shows that within this order of approximation, i. e. if three-spin-correlations and secondary effects brought about by them are systematically neglected, the only mechanism for the realization of short-range order in the Ising-model is given by the identity

$$\langle \mathbf{s}_m^+ \, \mathbf{s}_{m+\Delta}^z \, \mathbf{s}_{m+\Lambda}^z \, , \mathbf{s}_{m+l}^- \rangle = \tfrac{1}{4} \langle \mathbf{s}_m^+ \, , \mathbf{s}_{m+l}^- \rangle \quad \text{for } \mathbf{\Lambda} = \mathbf{\Delta} \tag{28}$$

which was taken into account in Chapters 2 and 3, but neglected in the derivations of the present chapter.

5. Evaluation and Discussion of the Thermodynamic Results

Now we return to the theory developed in Chapter 3. We evaluate and discuss the solutions resulting from Eqs. (20) – (22), and compare the results with those following from the two-spin-cluster molecular field approach.

For H vanishing Eq. (21) has the trivial solution $s = 0$ and, moreover, if $s(T)$ is one solution, $-s(T)$ is another one. These are rather elementary requisitions which must be claimed to hold for every reasonable theory on this subject [12].

The correlation in the unmagnetized phase which gives rise to short-range order above the transition point, follows from (21 b) to be

$$q = \frac{1}{4\sqrt{z}} \tanh\left(\frac{\beta J \sqrt{z}}{2}\right), \tag{29 a}$$

an expression which is in concurrence with

$$q = \tfrac{1}{4} \tanh\left(\frac{\beta J}{2}\right) \tag{29 b}$$

for the two-spin-cluster theory and with $q = 0$ according to Weiss.

For $T \to \infty$ and all values of H the magnetization and short-range order vanish in correspondence with the exact results.

In the limit of $\beta \to \infty$ i. e. $T \to 0$ there exists a non-trivial solution $s = -1/2$ and $q = 1/4$ which persists for $H = 0$ and gives rise to the phase transition discussed below. For very low temperatures this solution behaves like

$$s = -\tfrac{1}{2} + \left(\frac{z+1}{z-1}\right)^2 e^{-\beta J z} \tag{30 a}$$

in contrast with the two-spin-cluster and the Weiss molecular field theories, both yielding asymptotically the exact result

$$s = -\tfrac{1}{2} + e^{-\beta J z} . \tag{30 b}$$

This non-trivial solution breaks down at the Curie-temperature T_C which in the usual manner may be derived by expanding Eq. (20 a) into a power series in s. Setting

$$\beta J(z-1) = K , \tag{31 a}$$
$$\cosh(\beta J \sqrt{z}) = C_0 , \quad \sinh(\beta J \sqrt{z}) = S_0 ,$$

we get from (21) and (22 a) the first terms of this expansion

$$\left[K^2\left(1 - \frac{K}{3!}\right) + \frac{(z-1)^2}{2z}\left(2 S_0 \sqrt{z}\,\beta J - (z+1)\, C_0 \beta J + \frac{z+1}{\sqrt{z}} S_0\right)\right] s^2 + O(s^4) = -\left[2 - K + 2 C_0 - \frac{z+1}{\sqrt{z}} S_0\right] \tag{31 b}$$

In the limit of $s \to 0$ the expression on the right hand must vanish. Hence the relation

$$2 - (z-1)\,\beta_C J + 2\cosh(\beta_C J \sqrt{z}) - \frac{z+1}{\sqrt{z}} \sinh(\beta_C J \sqrt{z}) = 0 \tag{32}$$

follows which determines the transition point

$$T_C = 1/k\,\beta_C .$$

The counterparts to this equation in the two-spin-cluster and Weiss molecular field theories are given by the simpler relations

$$1 - (z-1)\,\beta_C J + e^{-\beta_C J} = 0 \tag{33 a}$$

respectively

$$\beta_C J = 2/z . \tag{33 b}$$

In the neighbourhood of T_C the magnetization vanishes like

$$s = \alpha \sqrt{T_C - T} , \tag{44}$$

as it does also in the other theories mentioned.

The transition points numerically evaluated from Eq. (32) for different lattice types are given in

[12] There is another asymptotic relation which must be fulfilled by every reasonable approximation: For $z = \infty$ the WMF becomes the exact description of the model [13] and therefore the results of all approximations must tend to it in the limit of $z \to \infty$. The proof for the approach of this paper is given in Appendix 2.

[13] F. BITTER, Introduction to Ferromagnetism, McGraw-Hill, New York 1937, p. 153.

	z	l. ch. 2	quadr. 4	triangle 6	s. c. 6	b. c. c. 8	f. c. c. 12
I	WMF	1	2	3	3	4	6
	2-sp.-cl.	0.782	1.888	2.923	2.923	3.941	5.960
	Eq. (32)	0.619	1.645	2.653	2.653	3.656	5.660
	BP-MF	0	1.442	2.466	2.466	3.476	5.484
II	series	0	1.134	1.824	2.256	3.176	4.896
	exact	0	1.134	1.821	?	?	?

Table 1. The transition points for several Ising lattices in different approximations. I: overall-approximations, II: special Ising-model methods. l. ch.: linear chain; quadr.: quadratic plane; triangle: hexagonal plane; s. c.: simple cubic; b. c. c.: body center cubic and f. c. c.: face centered cubic lattice. WMF: Weiss molecular field theory; 2-sp.-cl.: two-spin-cluster approach; Eq. (32): theory of this paper; BP-MF: BETHE-PEIERLS molecular field theory [14, 15]; series: high temperature expansions for the susceptibility [9]; exact: according to ONSAGER [16] and YANG [17].

Table 1 in comparison with the results of several other calculation methods.

As is seen from this table the transition points derived from (32) compared with those evaluated from the two-spin-cluster theory tend considerably towards lower temperatures, i. e. into the right direction, but they are always higher than the results which BETHE [14] and PEIERLS [15] have derived from a $(z+1)$-spin-cluster molecular field theory. In contrast to this approach our derivation incorrectly yields a phase transition for the linear chain, and, in agreement with it, it does not take into account the topological structure of the lattice: for the triangle and the simple cubic lattice – both with $z=6$ – we get the same Curie-point. As already suspected the largest discrepancies in comparison with the results of exact calculations and series expansions are found for the hexagonal plane and the face centered cubic lattices, where additional correlation effects, coming from the fact that in these lattice types the nearest-neighbours of one site may be adjoining one another, are neglected in our approach.

In Fig. 2 we compare the results of our approximation with those of the WMF, as evaluated for the s. c. lattice. The most important difference in comparison with this approach lies in the existence of short-range order for $T>T_C$, but the nearest-neighbour-correlation q shows a break at the transition point instead of a singularity in scope, as it exactly should be [18].

For low temperatures ($T \lesssim T_C/2$) s^2 is a good approximaton for the correlation q.

In Fig. 3 the same results are plotted in comparison with the curves evaluated from the two-spin-cluster molecular field theory. Apart from the improvement in the transition point, mentioned above,

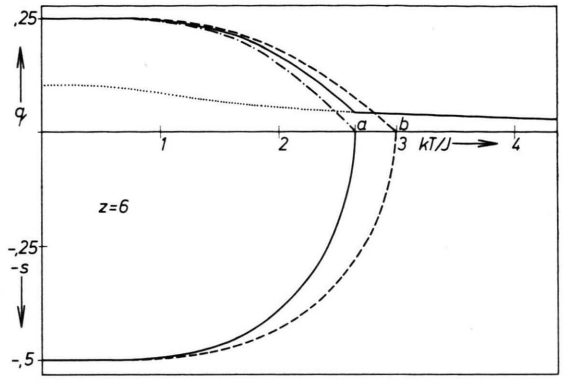

Fig. 2. Comparison of the results of the present approach with WMF for the s.c. lattice. ————: s and q from Eqs. (20), – – – –: s and q after WMF, —·—·—: s^2 after Eq. (20), ·····: correlation in the unmagnetic phase [Eq. (29 a)]. a: Curie point according to (32), b: Curie point according to WMF.

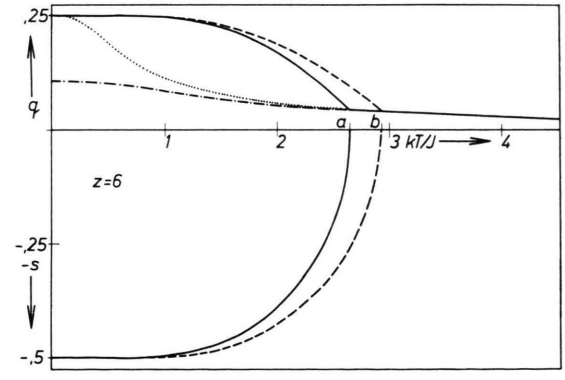

Fig. 3. Comparison of the results of the present approach with the two-spin-cluster molecular field theory for the s.c. lattice. ————: s and q from Eqs. (20), – – – –: s and q from Eqs. (A 5), —·—·—: q in the unmagnetic phase after (29 a), ·····: the same quantity in the two-spin-cluster-approach. a: Curie point according to (32), b: Curie point of the two-spin-cluster theory.

the most obvious difference of the two approaches is in the asymptotic behaviour of the correlation in the unmagnetic phase for low temperatures: q tends

[14] H. A. BETHE, Proc. Roy. Soc. London A **150**, 552 [1935].
[15] R. E. PEIERLS, Proc. Cambridge Phil. Soc. **32**, 471 [1936].
[16] L. ONSAGER, Phys. Rev. **65**, 117 [1944].
[17] C. N. YANG, Phys. Rev. **85**, 809 [1952].
[18] This break appears in all overall-approximations.

towards $1/4\sqrt{z}$ in our theory in contrast to the molecular field approach which yields $q \to 1/4$. But this behaviour is without further physical relevance, because this phase is unstable for thermodynamic reasons.

Apart from these differences both theories yield very similiar results, especially as to the low temperature behaviour of s and q and to the short-range order above the transition point.

For the last point we shall account for the paramagnetic susceptibility in this region. By implicit differentiation of Eq. (21) we get the formula

$$\chi = \left.\frac{\mathrm{d}s}{\mathrm{d}H}\right|_{s,\,H=0} = \frac{-\beta}{2-\beta J(z-1)+2\cosh(\beta J\sqrt{z})-\frac{z+1}{\sqrt{z}}\sinh(\beta z\sqrt{z})}. \tag{34 a}$$

In it for $T = T_C$ the denominator vanishes due to (32), so that χ in the correct way becomes singular at the transition point. For high temperatures (34 a) tends asymptotically to

$$\chi_{as} = \frac{-\beta}{2/2-\beta J z} \tag{34 b}$$

which is exactly the Curie-Weiss-law resulting from WMF. For temperatures above, but near to T_C, deviations from this simple law appear in (34 a) which are a direct consequence of the onset of short-range order in this temperature interval.

6. Conclusions

As we have seen from the preceding discussion the natural reference point for a comparison of the theory presented in this paper is given by the Oguchi type two-spin-cluster molecular field approximation for the Ising-model. There is a good agreement of the results of both approaches for low and high temperatures, but in the critical region our theory seems to present a real improvement because of the more accurate values for the transition point, it yields.

On the other hand not only by inspection of the results, but also from theoretical considerations our theory and that of Oguchi are closely related. This is due to the fact that in both approaches two-particle-correlations are the only ones involved, and all higher correlations are systematically neglected. In contrast to this e. g. in the Bethe-Peierls theory such higher correlations are taken into account.

[19] J. S. SMART, Effective Field Theories of Magnetism, W. B. Saunders Company, Philadelphia 1966.

The difference of the two approaches compared, and with it the key for an understanding of the different quality of their results, lies in the fact, that in Oguchi's theory only the correlation within one fixed two-spin-cluster is considered, whereas in our approximation all pairs of nearest-neighbours contribute to the correlation in a highly symmetrical way. The decoupling needed for a separation of the two- from the more-particle-correlations in this case is provided by a very plausible generalization of the successful procedure invented by Tjablikov.

A very important question is that one concerning the possibility of a generalization of the method adopted in this paper to the Heisenberg-model. On one hand, as we have already emphasized, Tjablikov's collective approach is essentially a single particle theory which by this fact cannot give adequate consideration to correlation effects. On the other hand the OGUCHI [3] and P. R. WEISS [4] molecular field approximations for the Heisenberg-model take into account cluster-correlations, but are local theories from the beginning which pretend an energy gap in the spectrum of the elementary excitations and therefore yield wrong results for the mathematical type of the temperature dependence of the magnetization at very low temperatures. Clearly it would be highly desirable to incorporate both correlations and the collective behaviour of the model in one approximation which should be expected to give the best overall-description of the Heisenberg-model available so far.

Indeed, as preliminary calculations have shown, it is possible by the method of correlation functions to bring together both features of the model in one system of differential equations, at least in a certain generalization of Oguchi's two-spin-cluster theory. But unfortunately in the evaluation of this system great mathematical difficulties arise which are neither completely understood in their origin nor overcome at present.

Acknowledgement

The opportunity of using the computer of the Rechenzentrum der Universität Kiel for the numerical evaluation of the theory is gratefully acknowledged.

Appendix

1. Concise Derivation of the Two-Spin-Cluster Molecular Field Theory for the Ising-Model

The derivation given in this appendix is completely based on the concepts of the molecular field approximation, as presented e. g. by SMART [19].

Let us investigate the statistical behaviour of an Ising-coupled cluster, consisting of two spins *0* and *1* under the influence of an effective magnetic field H_{eff} which is given by

$$H_{\text{eff}} = H' - 2J(z-1)s\,. \tag{A 1}$$

The Hamiltonian of this cluster is

$$\boldsymbol{H} = -2J\,\boldsymbol{s}_0{}^z\,\boldsymbol{s}_1{}^z + H_{\text{eff}}(\boldsymbol{s}_0{}^z + \boldsymbol{s}_1{}^z) \tag{A 2}$$

and the statistical quantities in question are defined by the following relations

$$s = \langle \boldsymbol{s}_0{}^z \rangle = \langle \boldsymbol{s}_1{}^z \rangle = -\frac{1}{2}\frac{\partial}{\partial(\beta H_{\text{eff}})}\,(\log \text{Trace}\, e^{-\beta \boldsymbol{H}})\,, \tag{A 3a}$$

$$q = \langle \boldsymbol{s}_0{}^z\,\boldsymbol{s}_1{}^z \rangle = \frac{\partial}{\partial(2J\beta)}\,(\log \text{Trace}\, e^{-\beta \boldsymbol{H}})\,. \tag{A 3b}$$

The trace

$$\text{Trace}\, e^{-\beta \boldsymbol{H}} = \sum_i e^{-\beta E_i} \tag{A 4}$$

is easily evaluated, because $\boldsymbol{H}$ has only the 4 eigenvalues

$$E_1 = -J/2 - H_{\text{eff}}\,, \quad E_{2,3} = J/2\,, \quad E_4 = -J/2 + H_{\text{eff}}\,.$$

Introducing them into (A 4) and performing the differentiations (A 3), one immediately gets the final expressions

$$s = -\frac{1}{2}\frac{\sinh(\beta H_{\text{eff}})}{\cosh(\beta H_{\text{eff}}) + e^{-\beta J}}\,, \tag{A 5a}$$

$$q = \frac{1}{4}\frac{\cosh(\beta H_{\text{eff}}) - e^{-\beta J}}{\cosh(\beta H_{\text{eff}}) + e^{-\beta J}} \tag{A 5b}$$

which together with the definition of H_{eff} (A 1) form a complete non-linear system for the evaluation of the magnetization s and the correlation q.

2. The Asymptotic Behaviour of the Theory in the Limit $z \to \infty$

As BITTER [13] has noted, the WMF becomes the exact theory of the Hamiltonian (1) in the limit of $z \to \infty$. This statement yields and additional boundary condition which must be met by every reasonable approximation for the Ising-model and which now is proved to be fulfilled by the approach of this paper at least in the limit of vanishing magnetic field.

If we go back to Eqs. (19) and (22) we find the asymptotical expressions

$$\nu \approx s\,z\,, \quad H_{\text{eff}} \approx -J\,z\,s \tag{A 6}$$

which, introduced into (21) and (22b) yield the result

$$s = \frac{\sinh(\beta J z s)}{2\cosh(\beta J z s) + [2\cosh(\beta J z s) - (1/s \cdot \sinh(\beta J z s))]}\,. \tag{A 7a}$$

This relation may be easily transformed into

$$4\cosh(\beta J z s)\cdot s - \sinh(\beta J z s) = \sinh(\beta J z s) \tag{A 7b}$$

which is exactly the WMF equation

$$s = \tfrac{1}{2}\tanh(\beta J z s)\,. \tag{A 7c}$$

For the correlation q we find from Eq. (20b)

$$\begin{aligned}\frac{q}{s} &= \frac{1}{4As}\{2s + 2sAC + 2sAS - 1 + AC - AS\} \\ &= \frac{1}{4As}\{4s - 1 + A^2\}\,,\end{aligned} \tag{A 8a}$$

and introducing (A 7c) into this equation we get

$$\frac{q}{s} = \tfrac{1}{2}\cdot\tanh(\beta J z s) = s\,, \tag{A 8b}$$

the result of Weiss' one-spin-cluster approach.

Therefore for $H = 0$ our approximation meets the boundary condition in the same way, as Oguchi's, Bethe-Peierls-Weiss' or Bogoljubov-Tjablikov's theories do.