SPECTRAL DENSITY APPROACH TO TRANSVERSE ISING PARAMAGNET

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An Ising model in a transverse field with general spin S is considered by spectral density approach in the unordered region. Expressions for the temperature renormalized excitation spectrum, the one-particle transverse correlation function, and the critical exchange-field ratio, are derived in two versions. At $T = 0$K expansions for thermodynamical quantities are given in the limit of weak interaction and critical ratios are calculated for several values of S.

1. *Introduction*

The $S = 1/2$ Ising model with transverse field has been a topic of investigation for about ten years. It describes the magnetic properties of singlet-singlet group state systems, and those of hydrogen bonded ferroelectrics and cooperative Jahn-Teller systems (Refs [1, 2] and references therein). Theoretical calculations by means of the first order Green-function method were performed by Wang and Cooper [3, 4], and Pink [5], whereas the perturbation expansion method has been applied for zero and low temperatures in Refs [6, 7], respectively. Expansions in powers of the high-density parametrs $1/z$ are given in the papers of Stinchcombe [1, 8] and Shender [9]. Recently, Refs [10–12], the methods of moments were used and agreement with the perturbation technique results was achieved. Critical values obtained by various authors are compared and results in Pink's decoupling are estimated by Popielewicz [13].

In the preceding paper [14], we considered the Ising model with transverse field for general spin S in the paramagnetic region within the Green-function method in the random-phase approximation. In the present paper, we propose a spectral density approach to this model. General expressions in the two versions for the thermodynamical quantities are obtained and zero-temperature characteristics are given explicitly. The structure of this paper is the following: Section 2 includes some definitions and expressions for the Green functions, as well as an expression for the temperature renormalized energy

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spectrum; in Section 3, the relations for the one-particle correlation function in the field direction and the critical ratio of the exchange interaction (the transverse fiedl upwards of which the paramagnetic phase is unstable) are derived; in Section 4, zero-temperature results are given in detail. Finally (Section 5), we discuss our results and check the self-consistency of the calculations.

2. *Green functions*

We consider the Hamiltonian of the transverse Ising model of the form

$$H = -\Delta \sum_j \hat{S}_j^z - 4\Gamma \sum_{l=m} J^{lm} \hat{S}_l^x \hat{S}_m^x, \tag{2.1}$$

where $\hat{S}_i^\alpha(\alpha = x, y, z)$ is the spin operator for the ion at the lattice site i; J^{ij}—the positive exchange integral between ions at sites i and j; Δ and Γ are constants of the model. The exchange integral is a function of the distance between the ions, and is restricted to nearest neighbours only.

We shall use the method of Zubarev's temperature-dependent commutator Green functions (Ref. [15]). The Green function $\langle\langle \hat{A}(t)|\hat{B}\rangle\rangle$ and its Fourier transform $\langle\langle \hat{A}|\hat{B}\rangle\rangle_E$ are defined as

$$\langle\langle \hat{A}(t)|\hat{B}\rangle\rangle = -i\theta(t)\langle[\hat{A}(t), \hat{B}]\rangle \tag{2.2}$$

$$\langle\langle \hat{A}|\hat{B}\rangle\rangle = \int_{-\infty}^{\infty} dt \langle\langle \hat{A}(t)|\hat{B}\rangle\rangle e^{iEt}, \tag{2.3}$$

respectively. The Green function $\langle\langle \hat{A}|\hat{B}\rangle\rangle_E$ fulfils the following equation of motion:

$$E\langle\langle \hat{A}|\hat{B}\rangle\rangle_E = \langle[\hat{A}, \hat{B}]\rangle + \langle\langle[\hat{A}, \hat{H}]|\hat{B}\rangle\rangle_E. \tag{2.4}$$

The spatial Fourier transforms $\hat{S}_k^\pm$ and $\hat{S}_k^z$ of the spin operators $\hat{S}_m^\pm$ and $\hat{S}_m^z$

$$\hat{S}_k^\pm = \sum_j \hat{S}_j^\pm e^{\mp ikj} \tag{2.5}$$

$$\hat{S}_k^z = \sum_j \hat{S}_j^z e^{ikj} \tag{2.6}$$

satisfy the following commutation relations

$$[\hat{S}_k^+, \hat{S}_{k'}^-] = 2\hat{S}_{-k+k'}^z \tag{2.7}$$

$$[\hat{S}_k^\pm, \hat{S}_{k'}^z] = \mp \hat{S}_{k\mp k'}^\pm. \tag{2.8}$$

The Hamiltonian (2.1), expressed in terms of the spatial Fourier transforms $\hat{S}_k^\pm$ and $\hat{S}_k^z$, is of the form

$$\hat{H} = -\Delta\hat{S}_0^z - \frac{\Gamma}{N}\sum_\kappa J(\kappa)(2\hat{S}_\kappa^+\hat{S}_\kappa^- + \hat{S}_\kappa^-\hat{S}_{-\kappa}^- + \hat{S}_\kappa^+\hat{S}_{-\kappa}^+), \tag{2.9}$$

where

$$J(k) = \sum_m J^{lm} e^{ik(l-m)}. \tag{2.10}$$

The operators $\hat{S}_k^{\pm}$ fulfil the equation of motion

$$i\dot{\hat{S}}_k^{+} = [\hat{S}_k^{+}, \mathscr{H}] = \Delta \hat{S}_k^{+} - \frac{4\Gamma}{N} \sum_{\kappa} J(\kappa) \hat{S}^z_{\kappa-k}(\hat{S}_\kappa^{+} + \hat{S}_{-\kappa}^{-}) \tag{2.11}$$

$$i\dot{\hat{S}}_k^{-} = [\hat{S}_k^{-}, \hat{\mathscr{H}}] = -\Delta \hat{S}_k^{-} + \frac{4\Gamma}{N} \sum_{\kappa} J(\kappa) \hat{S}^z_{k-\kappa}(\hat{S}_{-\kappa}^{+} + \hat{S}_\kappa^{-}). \tag{2.12}$$

We linearize the equations of motion of the spin operators $\hat{S}_k^{\pm}$ to the form

$$[\hat{S}_k^{+}, \mathscr{H}] = \Omega_{11}^k \hat{S}_k^{+} + \Omega_{12}^k \hat{S}_{-k}^{-} \tag{2.13}$$

$$[\hat{S}_{-k}^{-}, \hat{\mathscr{H}}] = -\Omega_{12}^k \hat{S}_k^{+} - \Omega_{11}^k \hat{S}_{-k}^{-}, \tag{2.14}$$

where the coefficients Ω_{11}^k and Ω_{12}^k will be defined within the spectral density method [16, 17] rather than by explicit RPA-like procedure. We introduce, after Ref. [17], the matrix Green function $G_k(E)$ and matrix spectral density function $\Phi_k(E)$, where

$$G_k(E) = \begin{pmatrix} \langle\langle \hat{S}_k^{+} | \hat{S}_k^{-} \rangle\rangle & \langle\langle \hat{S}_k^{+} | \hat{S}_{-k}^{+} \rangle\rangle \\ \langle\langle \hat{S}_{-k}^{-} | \hat{S}_k^{-} \rangle\rangle & \langle\langle \hat{S}_{-k}^{-} | \hat{S}_{-k}^{+} \rangle\rangle \end{pmatrix} \tag{2.15}$$

$$\Phi_k(E) = -\frac{1}{\pi} \operatorname{Im} G_k(E + i\varepsilon). \tag{2.16}$$

If we want to conserve, within first order Green-function theory, two moments of the spectral density $\Phi_k(E)$ (for details see Refs [16, 17]), then

$$\Omega_{11}^k = \langle [[\hat{S}_k^{+}, \hat{\mathscr{H}}], \hat{S}_k^{-}] \rangle / \langle [\hat{S}_k^{+}, \hat{S}_k^{-}] \rangle \tag{2.17}$$

$$\Omega_{12}^k = -\langle [[\hat{S}_k^{+}, \hat{\mathscr{H}}], \hat{S}_{-k}^{+}] \rangle / \langle [\hat{S}_k^{+}, \hat{S}_k^{-}] \rangle. \tag{2.18}$$

After straightforward commutations on the right hand side of Eqs (2.17) and (2.18), we obtain

$$\Omega_{11}^k = \Delta + \Omega_{12}^k \tag{2.19}$$

$$\Omega_{12}^k = \frac{2\Gamma J(0)}{\sigma N^2} \sum_{\kappa} \gamma_\kappa (\langle \hat{S}_\kappa^{-} \hat{S}_\kappa^{+} \rangle + \langle \hat{S}_\kappa^{-} \hat{S}_{-\kappa}^{-} \rangle - 2 \langle \hat{S}^z_{\kappa-k} \hat{S}^z_{k-\kappa} \rangle, \tag{2.20}$$

where

$$\gamma_k = J(k)/J(0) \tag{2.21}$$

$$\sigma = \langle S^z \rangle. \tag{2.22}$$

The following results are easily obtained from the standard procedure of Green-function theory

$$E_k = \sqrt{(\Omega_{11}^k)^2-(\Omega_{12}^k)^2}$$

$$= \Delta\left[1+\frac{A\alpha}{N}\sum_{\kappa}\frac{\gamma_\kappa}{(E_\kappa/\Delta)}\coth\frac{\beta E_\kappa}{2}-\frac{2A\gamma_k}{\sigma N^2}\sum_{\kappa}\gamma_\kappa\langle\hat{S}_\kappa^z\hat{S}_{-\kappa}^z\rangle\right]^{1/2} \tag{2.23}$$

$$\langle\hat{S}_k^-\hat{S}_k^+\rangle = N\sigma\left[\tfrac{1}{2}\left(\frac{\Delta}{E_k}+\frac{E_k}{\Delta}\right)\coth\frac{\beta E_k}{2}-1\right] \tag{2.24}$$

$$\langle\hat{S}_k^-\hat{S}_{-k}^-\rangle = N\sigma\,\tfrac{1}{2}\left(\frac{\Delta}{E_k}-\frac{E_k}{\Delta}\right)\coth\frac{\beta E_k}{2}, \tag{2.25}$$

where

$$A = 4\Gamma J(0)/\Delta \tag{2.26}$$

$$\alpha = \begin{cases}1 \text{ for OSDM (ordinary spectral density method [16])}\\ (\sigma/S)^2 \text{ for MSDM (modified spectral density method [18]).}\end{cases} \tag{2.27}$$

The value $(\sigma/S)^2$ of the parameter α follows from the replacement

$$1/\sigma \to \sigma/S^2 \tag{2.28}$$

in the first two components on the right hand side of Eq. (2.20). The relation (2.28) corresponds (Ref. [18]), in the case of the Green-function theory of isotropic Heisenberg ferromagnet, to Callen's decoupling. It is worth noting that $\sigma/S \neq 1$ even at $T = 0°$K due to zero-point motion. Expression (2.23) represents a transcendental equation for the collective excitation energy and includes two quantities: σ and $\langle\hat{S}_k^z\hat{S}_{-k}^z\rangle$, which have to be calculated in order to close the thermodynamics.

3. *Transverse correlation function*

We introduce after Haley and Erdös [19] standard-basis operators $\hat{L}_{\alpha\beta} = |\alpha\rangle\langle\beta|$ in the $\hat{S}^z$ representation, where

$$|\alpha\rangle \equiv |S, S-\alpha\rangle, \quad (\alpha = 0, 1, \ldots, 2S). \tag{3.1}$$

The spatial Fourier transforms $\hat{L}_{\alpha+1,\alpha}^k$

$$\hat{L}_{\alpha+1,\alpha}^k = \sum_m \hat{L}_{\alpha+1,\alpha}^m e^{ikm} \tag{3.2}$$

of the operators $\hat{L}_{\alpha+1,\alpha}$ fulfil the following commutation relations

$$[\hat{S}_k^+, \hat{L}_{\alpha+1,\alpha}^\kappa] = M_\alpha(\hat{L}_{\alpha\alpha}^{-k+\kappa}-\hat{L}_{\alpha+1,\alpha+1}^{-k+\kappa}) \tag{3.3}$$

$$[\hat{S}_k^-, \hat{L}_{\alpha+1,\alpha}^\kappa] = M_{\alpha+1}\hat{L}_{\alpha+2,\alpha}^{k+\kappa}-M_{\alpha-1}\hat{L}_{\alpha+1,\alpha-1}^{k+\kappa}, \tag{3.4}$$

where

$$M_\alpha = [S(S+1)-(S-\alpha)(S-\alpha-1)]^{1/2}. \tag{3.5}$$

We consider the Green functions $\langle\langle \hat{S}_k^+ | \hat{L}_{\alpha+1,\alpha}^k \rangle\rangle_E$ and $\langle\langle \hat{S}_{-k}^- | \hat{L}_{\alpha+1,\alpha}^k \rangle\rangle_E$. On solving the set of equations of motion (2.4) for our Green functions and using the condition that in the paramagnetic region

$$\langle [\hat{S}_{-k}^-, \hat{L}_{\alpha+1,\alpha}^k] \rangle \sim \langle (\hat{S}^-)^2 \rangle = 0 \tag{3.6}$$

we obtain

$$\langle\langle \hat{S}_k^+ | \hat{L}_{\alpha+1,\alpha}^k \rangle\rangle = \langle [\hat{S}_k^+, \hat{L}_{\alpha+1,\alpha}^k] \rangle \times \left[\tfrac{1}{2}\left(1+\frac{\Omega_{11}^k}{E_k}\right)\frac{1}{E-E_k} + \tfrac{1}{2}\left(1-\frac{\Omega_{11}^k}{E_k}\right)\frac{1}{E+E_k} \right], \tag{3.7}$$

$$\langle\langle \hat{S}_{-k}^- | \hat{L}_{\alpha+1,\alpha}^k \rangle\rangle = \langle [\hat{S}_k^+, \hat{L}_{\alpha+1,\alpha}^k] \rangle \left(-\frac{\Omega_{12}^k}{2E_k}\right)\left[\frac{1}{E-E_k} - \frac{1}{E+E_k}\right], \tag{3.8}$$

where we have decoupled the high-order Green functions according to Eqs (2.13) and (2.14). The quantities E_k, Ω_{11}^k and Ω_{12}^k are given by Eqs (2.23), (2.17) and (2.18), respectively. On the ground of the spectral theorem [15], the Green function (3.7) leads to

$$D_{\alpha+1} - \frac{\Phi}{1+\Phi} D_\alpha = 0, \tag{3.9}$$

where

$$D_\alpha = \langle \hat{L}_{\alpha\alpha} \rangle \tag{3.10}$$

$$\Phi = -\tfrac{1}{2} + \frac{1}{4N}\sum_k \left(\frac{E_k}{\Delta} + \frac{\Delta}{E_k}\right)\coth\frac{\beta E_k}{2}. \tag{3.11}$$

Finally (for details we refer the reader to the Ref. [14]), we obtain:

$$\sigma = \frac{(S-\Phi)(1+\Phi)^{2S+1} + (1+S+\Phi)\Phi^{2S+1}}{(1+\Phi)^{2S+1} - \Phi^{2S+1}}. \tag{3.12}$$

The two-particle correlation function $\langle \hat{S}_k^z \hat{S}_{-k}^z \rangle$ can be calculated approximately by means of RPA-like decoupling

$$\langle \hat{S}_k^z \hat{S}_{-k}^z \rangle \to \langle \hat{S}_k^z \rangle \langle \hat{S}_{-k}^z \rangle.$$

In this approximation, the expression for the collective excitation spectrum is of the form

$$\frac{E_k}{\Delta} = \left[1 - 2A\sigma\gamma_k + \frac{\alpha A}{N}\sum_\kappa \frac{\gamma_\mu}{(E_\kappa/\Delta)}\coth\frac{\beta E_\kappa}{2}\right]^{1/2}. \tag{3.13}$$

The set of selfconsistent Eqs (3.11), (3.12) and (3.13) describes the thermodynamics of our model and can in principle be solved numerically throughout the entire range of temperatures. These equations simplify at $T = 0°K$; nevertheless, the analytical expressions are available in the special weak interaction limit only. We present our zero-temperature results in the following section.

4. Zero-temperature results

At $T = 0°K$, Eqs (3.11) and (3.13) take the simpler form

$$\frac{E_k}{\Delta} = \left[1 - 2A\sigma\gamma_k + \frac{\alpha A}{N}\sum_{\kappa}\frac{\gamma_\kappa}{E_\kappa/\Delta}\right]^{1/2} \tag{4.1}$$

$$\Phi = -\tfrac{1}{2} + \frac{1}{4N}\sum_k\left(\frac{E_k}{\Delta} + \frac{\Delta}{E_k}\right). \tag{4.2}$$

The condition

$$2A\sigma - \frac{\alpha A}{N}\sum_{\kappa}\frac{\gamma_\kappa}{E_\kappa/\Delta} = 1 \tag{4.3}$$

determines a critical value A_c for which the gap at $\vec{k} = 0$ vanishes. For $A > A_c$ the gap becomes imaginary, indicating that the paramagnetic state is unstable and a transition to the ordered state occurs. At $A = A_c$

$$\frac{E_k}{\Delta} = \sqrt{2\sigma A_c}\sqrt{1-\gamma_k}\,. \tag{4.4}$$

On insertion of Eq. (4.4) into Eqs (4.2) and (4.3), we obtain by simple algebra

$$\Phi = -\tfrac{1}{2} + \tfrac{1}{4}\left[\sqrt{2\sigma A_c}\,\frac{1}{N}\sum_k\sqrt{1-\gamma_k} + \frac{1}{\sqrt{2\sigma A_c}}\,\frac{1}{N}\sum_k\frac{1}{\sqrt{1-\gamma_k}}\right] \tag{4.5}$$

$$\sqrt{A_c} = \frac{1}{\sqrt{2\sigma}}\left[\left(\frac{\alpha c}{2\sigma}\right) + \sqrt{\left(\frac{\alpha c}{2\sigma}\right)^2 + 4}\right]\Big/2, \tag{4.6}$$

where

$$c = \frac{1}{N}\sum_k\frac{\gamma_k}{\sqrt{1-\gamma_k}}. \tag{4.7}$$

The right-hand side of Eq. (4.6) depends on σ and the lattice sum c. Therefore, the quantity Φ is expressed by σ and we can solve Eq. (3.12) numerically. After that, by insertion of σ

into formula (4.6) we obtain A_c. Our expressions include standard lattice sums already calculated in the literature. We take, after Refs [3, 20],

$$\frac{1}{N}\sum_k \frac{1}{\sqrt{1-\gamma_k}} = \begin{cases} 1.111 \text{ for SC} \\ 1.084 \text{ for BCC} \\ 1.071 \text{ for FCC} \end{cases}$$

$$\frac{1}{N}\sum_k \sqrt{1-\gamma_k} = \begin{cases} 0.975 \text{ for SC} \\ 0.981 \text{ for BCC} \\ 0.986 \text{ for FCC} \end{cases}$$

The values of A_c for several values of S at $T = 0$ K are listed in Table I. In the particular case $S = 1/2$ our results agree with those of Wang and Cooper [3] in TSCA approximation (which corresponds to our MSDM approximation) and of Pfeuty and Elliott [6] in series expansion method (see also Ref. [13, 21, 22]).

TABLE I

Critical values A_c for cubic lattices, nearest neighbour interaction

S	Simple cubic		Body-centred cubic		Face-centred cubic	
	OSDM	MSDM	OSDM	MSDM	OSDM	MSDM
$\frac{1}{2}$	1.199	1.186	1.147	1.139	1.121	1.116
1	0.547	0.546	0.535	0.534	0.529	0.529
$\frac{3}{2}$	0.354	0.353	0.349	0.349	0.346	0.346
2	0.261	0.261	0.259	0.259	0.257	0.257
$\frac{5}{2}$	0.207	0.207	0.206	0.205	0.205	0.205
3	0.172	0.172	0.170	0.170	0.170	0.170

We can expand the right-hand side of Eq. (4.5) in terms of $(\alpha c/2\sigma) \ll 1$

$$\Phi = -\tfrac{1}{2}+\tfrac{1}{4}\left[\frac{1}{N}\sum_k \frac{2-\gamma_k}{\sqrt{1-\gamma_k}} - \left(\frac{\alpha c}{2\sigma}\right)\frac{1}{2N}\sum_k \frac{\gamma_k}{\sqrt{1-\gamma_k}} + \dots\right]. \tag{4.8}$$

If $S \to \infty$, then $(\alpha c/2\sigma) \to 0$. Therefore

$$\Phi(S = \infty) = -\tfrac{1}{2}+\frac{1}{2N}\sum_k \frac{1-\gamma_k/2}{\sqrt{1-\gamma_k}}. \tag{4.9}$$

The asymptotical expression (4.9) is identical with that of Ref. [14], obtained in RPA approximation. It can be easily shown that the asymptotical value of A_c also coincides with the RPA result

$$A_c \simeq 1/2S \tag{4.10}$$

as $S \to \infty$.

In the following, we consider the opposite limit of a weak interaction $SA \ll 1$. We solve the set of Eqs (4.1), (4.2) and (3.12) by means of an iterative method expanding E_k, Φ and σ in a power series in A up to order A^4/z^2. The quantity σ has, according to Callen (Ref. [23]), the following expansion in Φ

$$\sigma = S-\Phi+(2S+1)\Phi^{2S+1}+\ldots \tag{4.11}$$

We start the iterative procedure taking as the zero approximation $E_k/\Delta = 1$. Then, from Eqs (4.2) and (4.11), it follows that $\Phi = 0$ and $\sigma = S$.

We return to Eq. (4.1) and obtain, as a first approximation,

$$\frac{E_k}{\Delta} = \sqrt{1-2AS\gamma_k} \tag{4.12}$$

and appropriate expressions for Φ and σ. After a few rather tedious iterations, we obtain the following results:

$$\frac{E_k}{\Delta} = 1-AS\gamma_k-\frac{A^2S^2}{2}\left(\gamma_k^2-\frac{1}{Sz}\right)-\frac{A^3S^3}{2}\left(\gamma_k^2-\frac{3}{2Sz}\gamma_k\right)+\ldots \tag{4.13}$$

$$\sigma = S\left[1-\frac{A^2S}{4z}\left(1+\frac{A^2}{4z}-\frac{7}{2}\frac{SA^2}{z}+\frac{45}{4}\frac{S^2A^2}{z}\right)\right]+(2S+1)\left(\frac{A^2S^2}{4z}\right)^{2S+1}\delta_{S,1/2}. \tag{4.14}$$

In these calculations, we restricted ourself to the case of hypercubic lattice and took the relations

$$\frac{1}{N}\sum_k \gamma_k^2 = \frac{1}{z}, \tag{4.15}$$

$$\frac{1}{N}\sum_k \gamma_k^4 = \frac{3}{z^2}\left(1-\frac{1}{z}\right) \tag{4.16}$$

given e. g. by Stinchcombe in Ref. [8].

The expressions (4.13) and (4.14) enable us to calculate other thermodynamical quantities. The free energy is expressed by the formula

$$\langle\hat{\mathscr{H}}\rangle/N = -\Delta\sigma\left[1+\frac{A}{2N}\sum_k\frac{\gamma_k}{E_k/\Delta}\right]$$

$$= -\Delta\left\{S\left[1+\frac{A^2S}{4z}\left(1-\frac{A^2}{4z}-\frac{SA^2}{2z}+\frac{15}{4}\frac{S^2A^2}{z}\right)\right]+(2S+1)\left(\frac{A^2S^2}{4z}\right)^{2S+1}\delta_{S,1/2}\right\}. \tag{4.17}$$

It is worth noting that the expansions (4.13), (4.14) and (4.15) are independent of α. In the particular case $S = 1/2$ they agree very well with the results of the series expansions method (Ref. [6]) and high density method (Ref. [8]).

5. *Discussion*

We have analysed the thermodynamical properties of the general Ising model with transverse field in the paramagnetic region within the framework of the Green-function method. Expressions for the excitation energy spectrum, transverse correlation function and critical ratio were derived in two versions and zero-temperature results were proposed. They are shown to be independent of the parameter α in the weak interaction limit and dependent on α in the critical region $A \approx A_c$.

Replacing γ_k by 0 in Eq. (4.1), we obtain the mean-field results $\Phi = 0$ and $\sigma = S$ at $T = 0$ K. (There is no quantum-mechanical reduction of spin). The critical value A_c in this approximation is equal to $1/2S$. Corrections to that result due to zero-point fluctuations are appreciable. They attain 20% for spin one-half, but in RPA [14] amount to a few percent only.

It is worthwhile to check how well the condition

$$\langle(\hat{S}^-)^2\rangle = \frac{1}{N^2}\sum_k \langle \hat{S}_k^- \hat{S}_{-k}^- \rangle = 0 \tag{5.1}$$

is obeyed. In the weak interaction limit we obtain

$$\langle(\hat{S}^-)^2\rangle/S = \frac{A^2S^2}{z}\left(1 - \frac{1}{2S}\right) + 0(A^4) \ll 1. \tag{5.2}$$

For comparison, in RPA

$$\langle(\hat{S}^-)^2\rangle/S = A^2S^2/z + \ldots \ll 1. \tag{5.3}$$

It is evident that the condition (5.1) is very well justified for $S = 1/2$ in our present SDM calculations.

TABLE II

Values $\langle(\hat{S}^-)^2\rangle/S$ calculated at the critical point

	$S = 1/2$	$S = 1$	$S = 3/2$	$S = 2$	$S = 5/2$	$S = 3$
SC:						
OSDM	−0.0054	0.031	0.043	0.050	0.053	0.056
MSDM	0.0000	0.033	0.044	0.050	0.053	0.056
RPA	0.066	0.067	0.067	0.067	0.067	0.067
BCC:						
OSDM	−0.0032	0.024	0.033	0.038	0.041	0.042
MSDM	−0.0000	0.025	0.034	0.038	0.041	0.042
RPA	0.050	0.051	0.051	0.051	0.051	0.051
FCC:						
OSDM	−0.0024	0.020	0.028	0.031	0.034	0.035
MSDM	0.0000	0.021	0.028	0.031	0.034	0.035
RPA	0.042	0.042	0.042	0.042	0.042	0.042

At the critical point

$$\langle(\hat{S}^-)^2\rangle = \frac{\sigma}{2}\left[\frac{1}{\sqrt{2\sigma A_c}}\frac{1}{N}\sum_k \frac{1}{\sqrt{1-\gamma_k}} - \sqrt{2\sigma A_c}\frac{1}{N}\sum_k \sqrt{1-\gamma_k}\right]. \tag{5.4}$$

For comparison, in RPA

$$\langle(\hat{S}^-)^2\rangle = \frac{1}{4A_c}\frac{1}{N}\sum_k \frac{\gamma_k}{\sqrt{1-\gamma_k}}. \tag{5.5}$$

We present the numerical values $\langle(\hat{S}^-)^2\rangle/S$ in Table II. They are of the order 10^{-2}. It is obvious from the results of Table II that for $S = 1/2$ the condition (5.1) is very well fulfilled in our MSDM calculations.

REFERENCES

[1] R. B. Stinchcombe, *J. Phys.* **C6**, 2459 (1973).
[2] R. J. Birgenau, AIP Conf. Proc., *Magnetism and Magnetic Materials–1972*, American Institute of Physics, N. York 1973, Nr 10, p. 1664.
[3] Yu-Li Wang, B. R. Cooper, *Phys. Rev.* **172**, 539 (1968).
[4] Yu–Li Wang, B. R. Cooper, *Phys. Rev.* **185**, 696 (1969).
[5] D. A. Pink, *Phys. Rev. Lett.* **33**, 897 (1974).
[6] P. Pfeuty, R. J. Elliott, *J. Phys.* **C4**, 2370 (1971).
[7] R. J. Elliott, C. Wood, *J. Phys.* **C4**, 2359 (1971).
[8] R. B. Stinchcombe, *J. Phys.* **C6**, 2484, 2507 (1973).
[9] E. F. Shender, *Zh. Eksp. Teor. Fiz.* **66**, 2198 (1974).
[10] G. Kamieniarz, A. Popielewicz, R. Micnas, E. Szczepaniak, *Phys. Lett.* **A55**, 329 (1976).
[11] K. N. Pak, *Phys. Status Solidi* (b) **74**, 673 (1976).
[12] G. Kamieniarz, *Phys. Status Solidi* (b) **75**, K97 (1976).
[13] A. Popielewicz, *Phys. Status Solidi* (b) **72**, K169 (1975).
[14] G. Kamieniarz, *J. Phys.* **C9**, 4003 (1976).
[15] D. N. Zubarev, *Usp. Fiz. Nauk* **71**, 71 (1960).
[16] O. K. Kalashnikov, E. S. Fradkin, *Phys. Status Solidi* (b) **59**, 9 (1973).
[17] Yu. G. Rudoy, Appendix to monograph of S. W. Tyablikov, *Methods of Quantum Theory of Magnetism*, Nauka, Moskov 1975 (in Russian).
[18] G. Kamieniarz, *Physica* **A86**, 417 (1977).
[19] S. B. Haley, P. Erdös, *Phys. Rev.* **B5**, 1106 (1972).
[20] R. Micnas, *J. Phys.* **C9**, 3307 (1976).
[21] A. Yanase, Y. Takeshige, M. Suzuki, *J. Phys. Soc. Jap.* **41**, 1108 (1976).
[22] A. Oitmaa, M. Pliszke, *J. Phys.* **C9**, 2093 (1976).
[23] H. B. Callen, *Phys. Rev.* **130**, 890 (1963).