# THERMODYNAMICAL BEHAVIOUR OF THE TWO- AND THREE-DIMENSIONAL AMORPHOUS ISING MODEL

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We consider a two- and three-dimensional amorphous Ising ferromagnet with positive exchange integrals $I_{ij} = \langle I\rangle + \Delta I_{ij}$ in the zero field case assuming the fluctuations of $I_{ij}$ are stochastical and small. By means of a thermodynamical perturbation theory we obtain the change of the free energy $\Delta f(T)$ in comparison with the corresponding crystalline case ($I_{ij} = \langle I\rangle$). The changes of the entropy, specific heat, internal energy, magnetization and susceptibility are calculated and discussed. The structure fluctuations cause a decrease of $f(T)$, $m(T)$, and $\chi(T)$. The convergence of the perturbation series is tested in a special case. The amorphous Ising antiferromagnet in the two-sublattice model is considered briefly.

## *1. Introduction*

The one-dimensional amorphous Ising ferromagnet was investigated in [1] by means of thermodynamical perturbation theory for the case $S_i^z = \pm 1$ [2] and was compared with the results given by Fan and McCoy [3]. Contrary to the method by Fan and McCoy the perturbation theory is applicable to the two- and three-dimensional case, too. As in [1] we use the stochastical lattice model in which the spins are localized on the lattice sites and being coupled by stochastically fluctuating exchange integrals which we can write in the form $I_{ij} = \langle I_{ij}\rangle + \Delta I_{ij} \cdot \langle I_{ij}\rangle$ is the structure average of the exchange integrals and $\Delta I_{ij}$ is the deviation from this average due to the structure fluctuations.

The basic equation for our calculations is the difference between the free energy per spin for the amorphous system and the corresponding crystalline system which is given by

$$\Delta f(T, H) = f(T, H) - f_0(T, H) = -\Delta^2 \cdot z\langle I_{ij}\rangle^2 \frac{\beta}{2}\left[1 - \left(\frac{1}{z}\frac{\partial f_0(T, H)}{\partial \langle I_{ij}\rangle}\right)^2\right] \tag{1}$$

(see [1], [2]).

The subscript "0" denotes the corresponding crystalline system in which is $I_{ij} = \langle I_{ij}\rangle$. $z$ is the number of the next neighbours and $\Delta^2$ is defined as follows

$$\frac{\langle \Delta I_{ij} \Delta I_{kl}\rangle}{\langle I_{ij}\rangle^2} = \frac{\Delta^2}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{2}$$

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From (1) we obtain in the usual way the changes of the entropy $\Delta s$, specific heat $\Delta c$, internal energy $\Delta u$, magnetization $\Delta m$ and susceptibility $\Delta\chi$ per spin induced by the fluctuations of the exchange integrals.

From (1–4) in [1] follows that we need for our calculations the quantities $u_0(T)$, $m_0(T)$ and $\chi_0(T)$. We consider for the two-dimensional case the simple-quadratic lattice and for the three-dimensional one the face-centered cubic lattice. The formulae for $u_0(T)$ and $m_0(T)$ are exactly known in the two-dimensional case [4, 5]. For $\chi_0(T)$ are used the results of a Padé-approximation in [6]. In the three-dimensional case the expression for $u_0(T)$ is given by series expansions [7], $\chi_0(T)$ and $m_0(T)$ are given by Padé-approximations [6]. The calculations are done for a zero magnetic field.

The perturbational theory is not correct in the immediate vicinity of the Curie temperature for the corresponding crystalline system $T_c^{(0)}$. Moreover the magnitudes $u_0(T)$, $m_0(T)$, and $\chi_0(T)$ for the three-dimensional case are only approximately given in this region. Therefore we must omit the region near $T_c^{(0)}$ from our considerations. The smaller is $\Delta^2$, the closer we can approach to $T_c^{(0)}$, because $\Delta^2$ is the expansion parameter.

## *2. Results and discussions*

The results of our calculations are plotted in the figures 1–4. In the following we discuss and interpret the results for $\Delta f(T)$, $\Delta s(T)$, $\Delta c(T)$, $c(T)$, $\Delta u(T)$, $\Delta m(T)$, and $\Delta\chi(T)$ for the two- and three-dimensional Ising model.

1. $\Delta f(T)$, (Fig. 1).

The shift in free energy is smaller or equal zero for all temperatures. This is in agreement with the Bogolyubov theorem for amorphous magnetic systems [8], which states that always $f(T) \leqslant f_0(T)$. The shift in free energy for the two- (and three-)dimensional case has a minimum above the Curie temperature of the corresponding crystalline system $T_c^{(0)}$ and approaches zero for higher temperatures.

2. $\Delta s(T)$, (Fig. 1, 4).

With increasing temperatures $\Delta s(T)$ increases from zero to plus infinity near $T_c^{(0)}$. Above $T_c^{(0)}$ $\Delta s(T)$ is negative and goes to zero for $T \to \infty$. The increasing of $\Delta s(T)$ at low temperatures is caused by the fluctuations with $\Delta I_{ij} < 0$ because of the smaller exchange integrals the coupling of many spins is weaker and the magnetic disorder enlarges. At high temperatures the greater exchange integrals with $\Delta I_{ij} > 0$ give rise to an additional local magnetic order. In the vicinity of $T_c^{(0)}$ the used simple perturbation theory gives no real results. Remarkable, if we regard the results found for the three-dimensional case in the region $T/T_c^{(0)} = 0.95, \ldots, 1.02$ as physically unreasonable (broken line), then we can suppose a behaviour for $\Delta s(T)$ (plotted), which is very similar to the one-dimensional case [1]. But it is possible that the difference between the two- and three-dimensional case is caused by the used series expansions in the three-dimensional case.

3. $\Delta c(T)$, (Fig. 1)

With increasing temperatures $\Delta c$ increases from zero to plus infinity near $T_c^{(0)}$. Above $T_c^{(0)}$ $\Delta c$ is first negative goes then to positive values and approaches zero for $T \to \infty$. In the

vicinity of $T_c^{(0)}$ we find in the two- and three-dimensional case a singular behaviour, which follows from the perturbational theory and has no physical meaning. Outside this region $\Delta c(T)$ behaves analogous to the one-dimensional case.

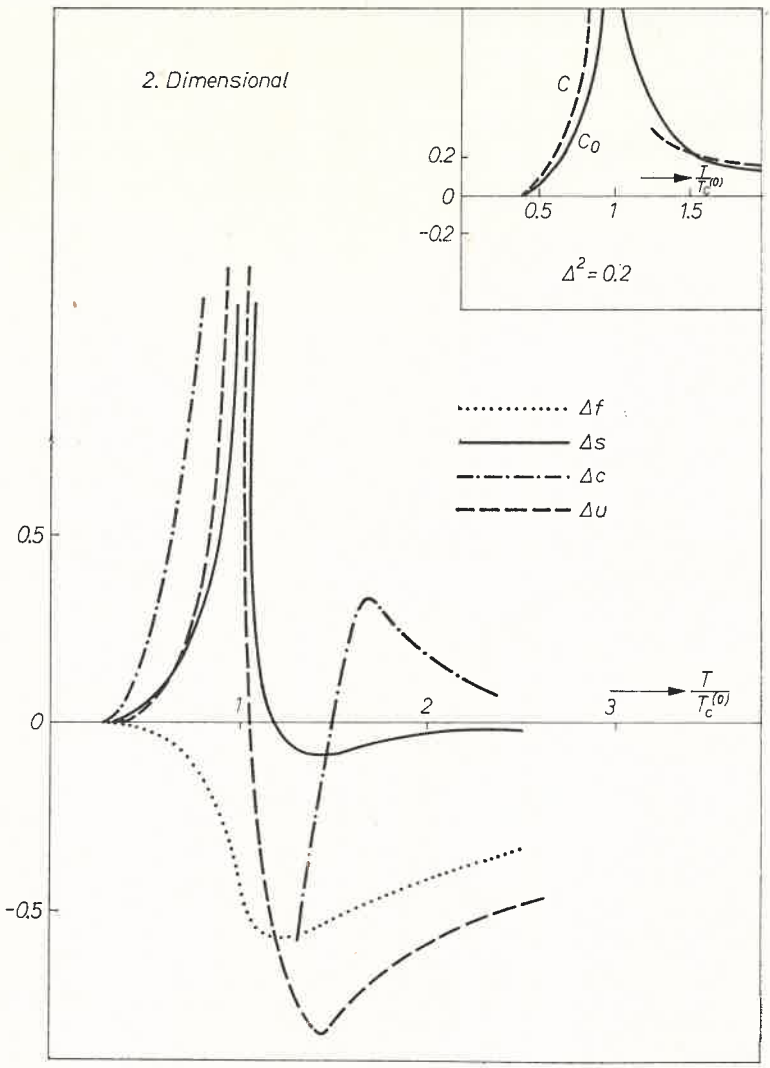


Fig. 1

4. $c(T)$, (Fig. 1)

With increasing temperatures $c(T)$ increases from zero to plus infinity near $T_c^{(0)}$. Above $T_c^{(0)}$ $c(T)$ decreases from plus infinity and approaches zero. In comparison to the crystalline case we notice a broadening of the peak away from the Curie temperature and

one can state a shift of the peak to lower temperatures. This suggests for the Curie temperature that $T_c < T_c^{(0)}$.

5. $\Delta u(T)$, (Fig. 1)

For $\Delta u(T)$ we find an analogous behaviour as in the one-dimensional case [1] (see also below *Remarks on the convergence*).

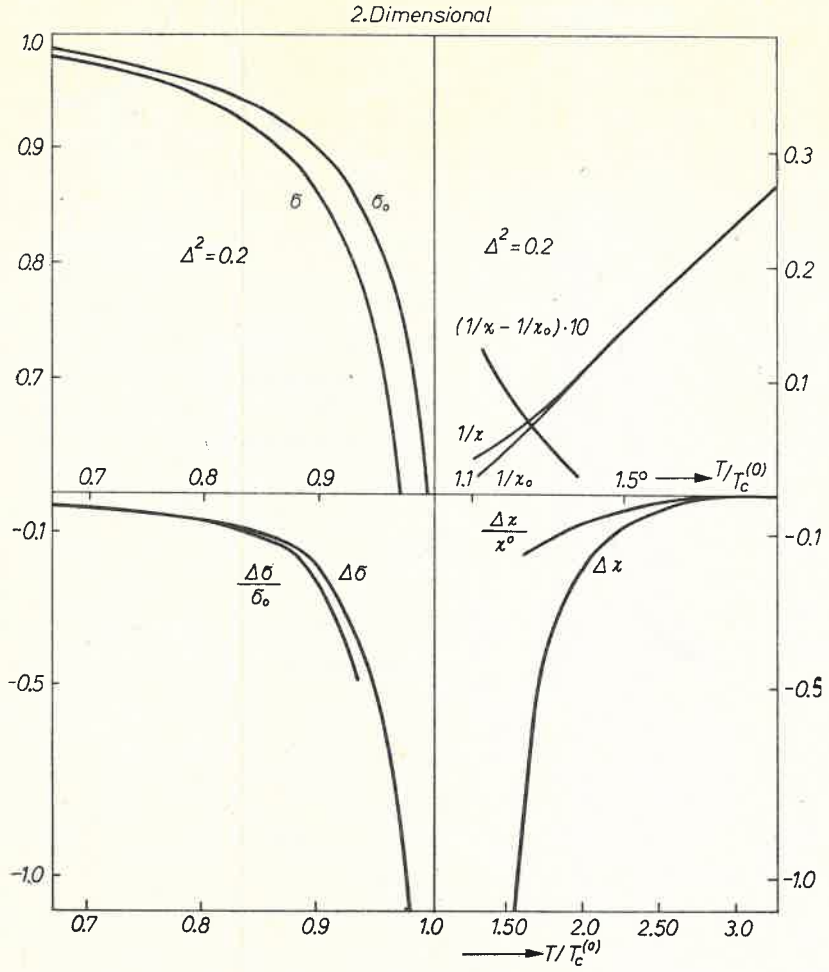


Fig. 2

6. $\Delta m(T), \Delta\chi(T)$, (Fig. 2, 3)

With increasing temperatures $\Delta m$ decreases from zero to minus infinity at $T_c^{(0)}$. Above $T_c^{(0)}$ $\Delta\chi$ increases from minus infinity and approaches zero. The changes of both the magnetization and susceptibility are in agreement with [2] always negative. This suggests also a shift of $T_c$ to lower temperatures. Remarkable that the relative changes of the magnet-

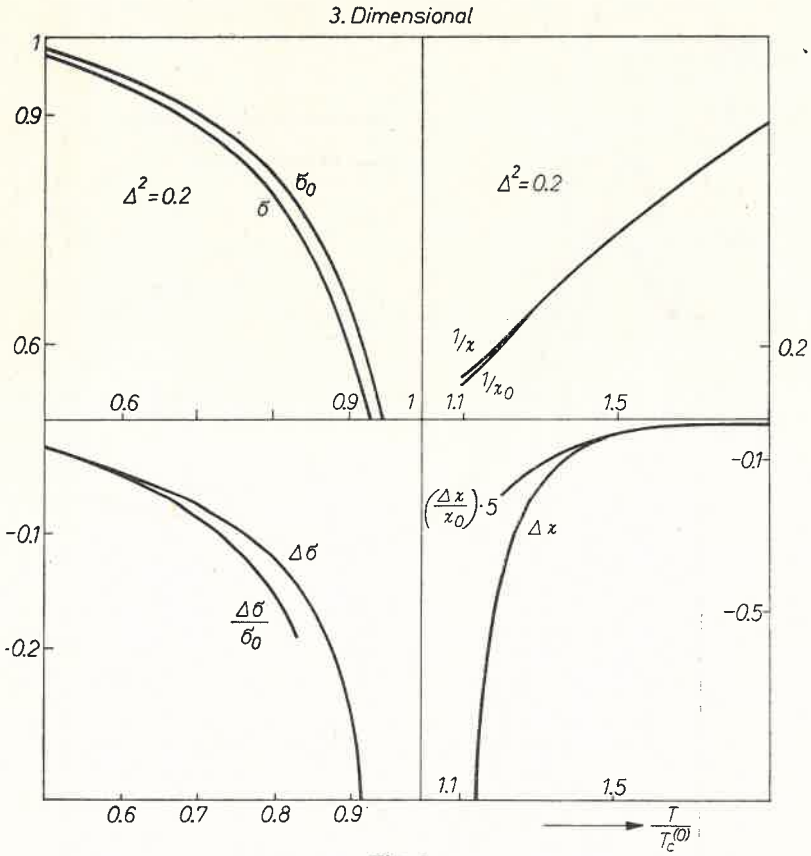
3. Dimensional
1
0.9
0.6
$\Delta^2=0.2$
$\sigma_0$
$\sigma$
0.6
0.9
1
$\Delta^2=0.2$
$1/\chi$
$1/\chi_0$
1.1
1.5
0.2
-0.1
-0.2
$\Delta\sigma$
$\frac{\Delta\sigma}{\sigma_0}$
0.6
0.7
0.8
0.9
$\left(\frac{\Delta\chi}{\chi_0}\right)\cdot 5$
$\Delta\chi$
-0.1
-0.5
1.1
1.5
$\frac{T}{T_c^{(0)}}$

Fig. 3

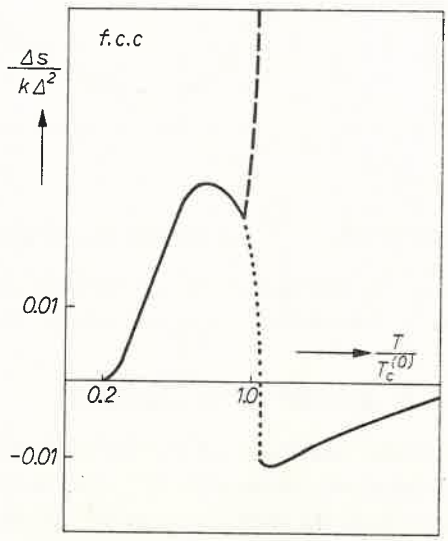
f.c.c
$\frac{\Delta s}{k\Delta^2}$
0.01
-0.01
0.2
1.0
$\frac{T}{T_c^{(0)}}$

Fig. 4

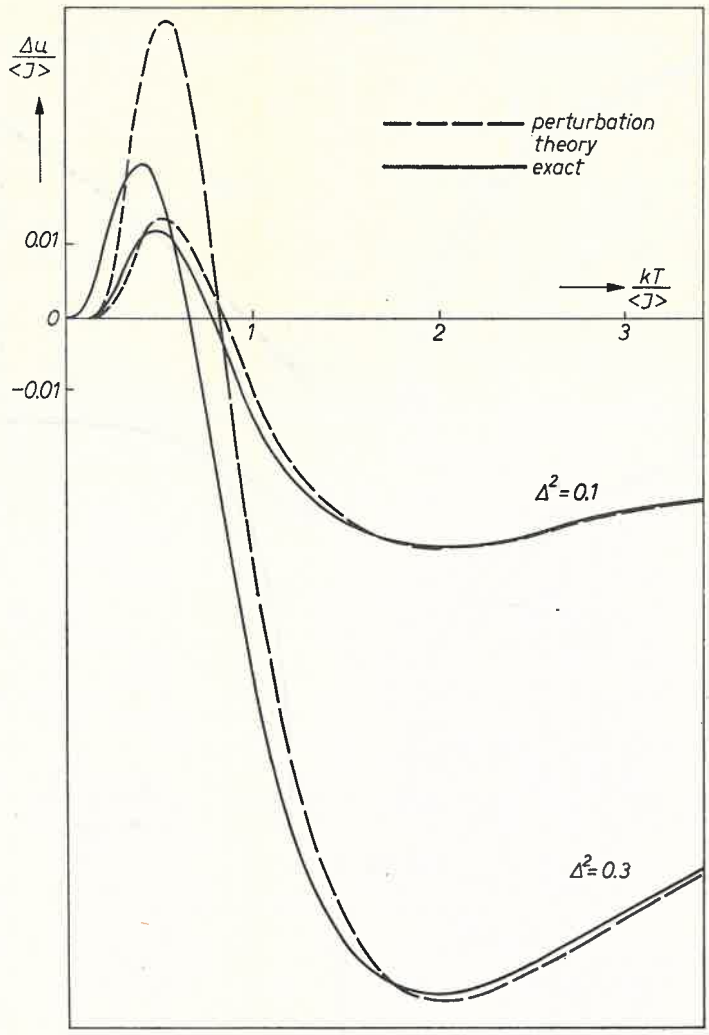


Fig. 5

ization $\frac{\Delta m}{m_0}$ and of the susceptibility $\frac{\Delta \chi}{\chi_0}$ are for the two-dimensional case greater than for the three-dimensional one. One can interpret this in the following way: The greater is the number of next neighbours $z$, the weaker is the influence of structure fluctuations.

### *3. Remarks on the convergence*

In every perturbation theory one must ask for the maximal perturbation parameter for which the calculation is physically reasonable. To verify this we consider for the one-dimensional amorphous Ising model the internal energy per spin for $H = 0$ (see Appendix). We assume a distribution function $w(I_{ij})$ for the stochastically fluctuating exchange integrals

$I_{ij}$. With it we calculate

$$\overset{\text{exact}}{\Delta u}(T, \Delta^2) = \overset{\text{exact}}{u}(T, \Delta^2) - u_0(T) = \int w(I_{ij}) \cdot u(T, I_{ij}) \cdot dI_{ij} - u_0(T) \tag{3}$$

and compare it with the change of the internal energy $\Delta u(T, \Delta^2)$ obtained by the perturbation theory. We regard various distribution functions $w(I_{ij})$. For all cases we find that with decreasing $\Delta^2$ $\Delta u(T, \Delta^2)$ approaches $\overset{\text{exact}}{\Delta u}(T, \Delta^2)$ (Fig. 5). From this we can conclude that our perturbational series reproduces the real situation in a good approximation for $\Delta^2 \lesssim 0.2$. In Fig. 5 one can see that with increasing temperatures this approximation is going better. One must remark that the tested zero field case is the most unfavourable case regarding the convergence of the perturbation series. Such a simple test of the convergence is not possible in the two- and three-dimensional case.

If we choose for a given distribution function the parameter $\Delta^2$ so great that by it a part of the exchange integrals is negative then we find a decreasing of the ground state energy (Fig. 6).

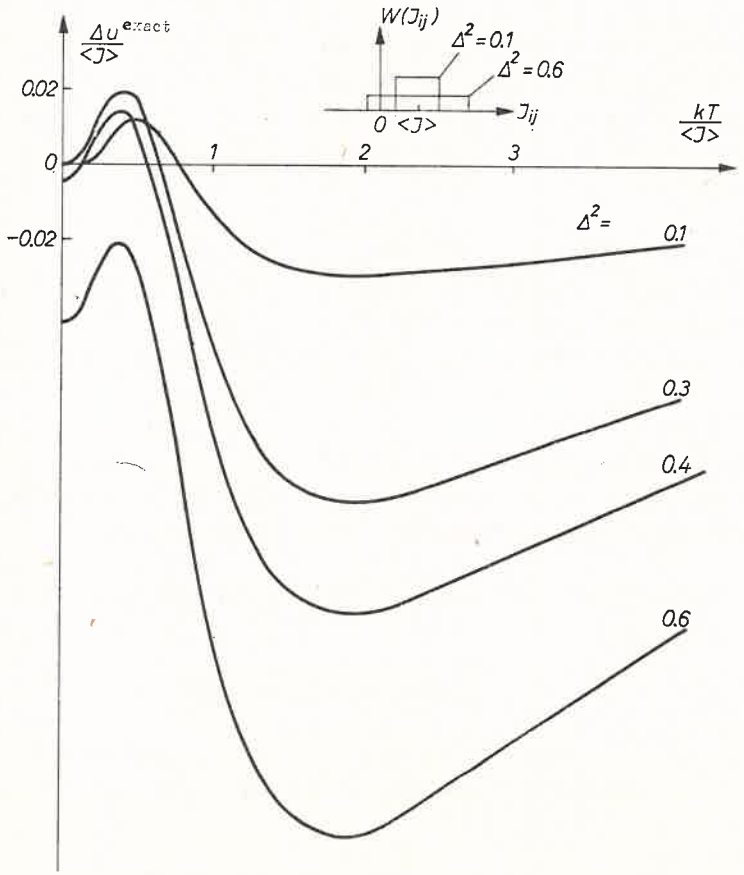


Fig. 6

### 4. *Antiferromagnetic case*

It is also possible without additional calculations to get the change in free energy for an amorphous Ising antiferromagnet in a zero magnetic field.

The free energy per spin of a crystalline Ising antiferromagnet with two sublattices and only next neighbour interactions is

$$f_0 = -\frac{1}{N}\frac{1}{\beta}\ln \sum_{\{S_A,S_B\}} e^{-\beta \sum_{i,j} |I_{ij}| S_i^z S_j^z}, \tag{4}$$

where $S_A$, $S_B$ denote the spins of the two sublattices. Obviously the substitution $S_B \to -S_B$ does not change the free energy $f_0$ (see also [9]). From this follows that for $H = 0$ the free energy is equal for an Ising antiferromagnet and for the corresponding ($I_{ij} \to -I_{ij}$) Ising ferromagnet. In an analogous way one can show the equality of the (sublattice) magnetization of the antiferromagnet and the magnetization of the corresponding ferromagnet for $H = 0$. From this one can conclude that $T_{\text{Neel}} = T_{\text{Curie}}$. The principal analogy between ferro- and antiferromagnetics holds also for arbitrary fluctuating exchange integrals within the lattice model. This means that all results for $\Delta f$, $\Delta s$, $\Delta u$, $\Delta c$, and $\Delta m$ for the amorphous Ising ferromagnet are the same for the two-sublattice amorphous Ising antiferromagnet (with next neighbour interaction) in the one-, two-, and three-dimensional case for $H = 0$. All this is also valid for the Heisenberg model, if the spin goes to infinity.

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## APPENDIX

The magnetic part of the partition function for the one-dimensional Ising chain in a zero magnetic field is given by

$$Z_{\text{St}} = \operatorname*{Tr}_{\{S_i,S_j\}} e^{\beta \sum_{ij} I_{ij} S_i^z S_j^z} = \operatorname*{Tr}_{\{S_i^z S_{i+1}^z\}} e^{2\beta \sum_i I_{i,i+1} S_i^z S_{i+1}^z} = \prod_i [4 \cosh (2\beta I_{i,i+1})],$$

where $S_i^z, S_j^z = \pm 1$.

The subscript "St" demonstrates the dependence from the arbitrary but fixed structure. Remarkable, in no wise we assume the same magnitude of the exchange integrals $I_{i,i+1}$. With this we obtain for the magnetic part of the free energy

$$F = \langle F_{\text{St}} \rangle = -\frac{1}{\beta} \ln Z_{\text{St}} = -\frac{1}{\beta} \langle \sum_i \ln (4 \cosh (2\beta I_{i,i+1})) \rangle =$$

$$= -\frac{N}{\beta} \langle \ln (4 \cosh (2\beta I_{i,i+1})) \rangle$$

where the operation $\langle \ldots \rangle$ means averaging with regard to the structure. Assuming any distribution of the exchange integrals $w(I_{i,i+1})$ the free energy per spin can exactly be written in the form

$$\overset{\text{exact}}{f(T)} = -\frac{1}{\beta} \cdot \int dI_{i,i+1} \cdot w(I_{i,i+1}) \cdot \ln (4 \cosh (2\beta I_{i,i+1})).$$

By it we get for the internal energy per spin

$$\overset{\text{exact}}{u(T)} = -2 \cdot \int dI_{i,i+1} \cdot w(I_{i,i+1}) \cdot I_{i,i+1} \cdot \tanh(2\beta I_{i,i+1}).$$

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