THE DOUBLE ISING CHAIN

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The thermodynamics of the simple spin model such as the double Ising chain in a zero field is given and the zero-field susceptibility is calculated.

1. Introduction

The interest in the theoretical investigation simple spin systems, among these also in one-dimensional models, persists to the present time. Such models, apart from their theoretical significance, are appropriate in the investigation of the magnetic properties of some compounds. In these compounds the magnetic ions are arranged in chains with strong interaction within each chain but rather weak interactions between chains.

In this paper we examine a certain version of the one-dimensional Ising model, for which the exact solution can be given. Our model consists of $2N$ "spins" arranged in

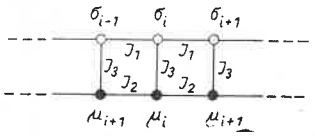

Fig. 1. The double Ising chain ($\sigma_i = \pm 1$, $\mu_i = \pm 1$)

a double chain, as represented in Fig. 1, and the interaction is limited to the nearest-neighbour pairs only.

The total energy of the system is given by

$$H_{2N} = -h \sum_i \sigma_i - h \sum_i \mu_i - J_1 \sum_i \sigma_i \sigma_{i+1} - J_2 \sum_i \mu_i \mu_{i+1} - J_3 \sum_i \mu_i \sigma_i \tag{1}$$

where h is the external field strength in suitable units, and J_1, J_2, J_3 are the exchange parameters.

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In a recent paper Kosevich and Galkin [1] considered the model of a double polymer chain with the Hamiltonian identical to (1) in order to study the phase transition corresponding to the denaturation of DNA. The phase transitions are possible in their model since appropriate statistical weights were chosen for the different states of a chain, according to the character of the denaturation process.

However, the simple "pure" Ising variant has not been considered in their paper. For such a simple case the thermodynamical functions in a zero magnetic field can be obtained by standard methods and it is also possible to examine them in relation to the character of interactions inside and between chains, which is the subject of the present paper.

The ends of the chain described by (1) may be treated in two different ways:

a) as free ends (the summation index $i = 1, 2, \ldots, N-1$),

b) as in a cyclic chain, when $i = 1, \ldots, N$ and

$$\sigma_{N+1} \equiv \sigma_1 , \quad \mu_{N+1} \equiv \mu_1 . \tag{2}$$

The partition function associated with (1) is

$$Z_{2N} = \sum_{\text{conf}} \exp(-\beta H_{2N}), \quad \left(\beta = \frac{1}{kT}\right). \tag{3}$$

The summation in (3) goes over all configurations of the system. The corresponding expression for the free energy taken per spin is

$$f_{2N} = -(2\beta N)^{-1} \ln Z_{2N}. \tag{4}$$

According to general results obtained by Griffiths [2] for a wide class of the spin systems, the following statements are valid in our case:

a) for arbitrary values of β ($\beta \neq 0$) and the parameters h, J_1, J_1, J_3 the sequence of functions f_{2N} is convergent

$$\lim_{N \to \infty} f_{2N} = f \tag{5}$$

here f is the free energy in the "thermodynamical limit",

b) f is independent on the conditions imposed on the ends of the chain.

Moreover, it can be easily proved (see also [2]) that:

c) if the functions f_{2N} are convex functions of some variable, then f is also convex,

d) the sequence of derivatives of the convex functions f_{2N} is convergent to the derivative of f, at every point where the derivative of f is continuous. Note, in addition, that if f_{2N} are odd (even) functions then f is also odd (even), respectively.

According to b) the most convenient boundary conditions can now be chosen in order to calculate the explicit form of f. Thus, for cyclic conditions, the free energy may be obtained with the aid of the transfer matrix method. This commonly used method (see, *e. g.*, [3]) has been already applied to study the one-dimensional Ising model with an arbitrary spin [4] which is similar, in some aspects, to the model described above.

2. The transfer matrix method

For cyclic boundary conditions the partition function Z_{2N} connected with (1), may be written as

$$Z_{2N} = \sum_{\text{conf.}} \prod_{i=1}^{N} \exp\left[\tfrac{1}{2}l(\sigma_i+\mu_i)+u\sigma_i\sigma_{i+1}+v\mu_i\mu_{i+1}+\right.$$

$$\left.+\tfrac{1}{2}w(\sigma_i\mu_i+\sigma_{i+1}\mu_{i+1})+\tfrac{1}{2}l(\sigma_{i+1}+\mu_{i+1})\right] \tag{6}$$

where

$$u \equiv \beta J_1, \quad v \equiv \beta J_2, \quad w \equiv \beta J_3, \quad l \equiv \beta h. \tag{7}$$

Further, after introducing the matrix $\mathscr{T}$ (the transfer matrix) with the matrix elements

$$\langle\sigma\mu|\mathscr{T}|\sigma'\mu'\rangle = \exp\left[\tfrac{1}{2}l(\sigma+\mu)+u\sigma\sigma'+v\mu\mu'+\tfrac{1}{2}w(\sigma\mu+\sigma'\mu')+\tfrac{1}{2}l(\sigma'+\mu')\right] \tag{8}$$

it is easily seen, that the partition function may be rewritten as

$$Z_{2N} = \mathrm{Tr}\mathscr{T}^N. \tag{9}$$

The matrix $\mathscr{T}$

$$\mathscr{T} = \begin{bmatrix} e^{2l+u+v+w} & e^{l-u+v} & e^{l+u-v} & e^{-u-v+w} \\ e^{l-u+v} & e^{u+v-w} & e^{-u-v-w} & e^{-l+u-v} \\ e^{l+u-v} & e^{-u-v-w} & e^{u+v-w} & e^{-l-u+v} \\ e^{-u-v+w} & e^{-l+u-v} & e^{-l-u+v} & e^{-2l+u+v+w} \end{bmatrix} \tag{10}$$

is, as usually, the symmetric real matrix, with real eigenvalues.

Besides, since the matrix elements are positive, there exists a positive eigenvalue λ_m, greater than the absolute values of the other eigenvalues, which is a single root of the secular equation (Perron's theorem, see *e. g.* [5]).

Thus

$$\lim_{N\to\infty} (Z_{2N})^{1/N} = \lambda_m \tag{11}$$

and

$$f = \lim_{N\to\infty} f_{2N} = -(2\beta)^{-1} \lim_{N\to\infty} \ln (Z_{2N})^{1/N} = -(2\beta)^{-1} \ln \lim_{N\to\infty} (Z_{2N})^{1/N} =$$

$$= -(2\beta)^{-1} \ln \lambda_m. \tag{12}$$

For $h = 0$ ($l = 0$ in (10)) the matrix $\mathscr{T}$ can be transformed to the quasi-diagonal form by the similarity transformation $\mathscr{T} \to \Omega\mathscr{T}\Omega^{-1}$,

$$\Omega = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix} = \Omega^{-1}. \tag{13}$$

In such a way, after solving simple quadratic equations, we obtain the eigenvalues:

$$\lambda_{1,2}(0) = 2(\mathrm{ch}(u+v)\,\mathrm{ch}\,w \pm \sqrt{\mathrm{ch}^2(u+v)\,\mathrm{sh}^2 w+\mathrm{ch}^2(u-v)}),$$
$$\lambda_{3,4}(0) = 2(\mathrm{sh}(u+v)\,\mathrm{ch}\,w \pm \sqrt{\mathrm{sh}^2(u+v)\,\mathrm{sh}^2 w+\mathrm{sh}^2(u-v)}). \tag{14}$$

It is easily seen that

$$\lambda_m(0) = \lambda_1(0) = 2(\mathrm{ch}(u+v)\,\mathrm{ch}\,w + \sqrt{\mathrm{ch}^2(u+v)\,\mathrm{sh}^2 w+\mathrm{ch}^2(u-v)}) \tag{15}$$

for every values of u, v, w.

When $w = 0$ (no interaction between chains) from (15) we obtain

$$\lambda_m(0) = 4\,\mathrm{ch}\,u\,\mathrm{ch}\,v. \tag{16}$$

Hence

$$f = -\tfrac{1}{2}(\beta^{-1}\ln 2\,\mathrm{ch}\,u+\beta^{-1}\ln 2\,\mathrm{ch}\,v) \tag{17}$$

as would be expected, if we compare (17) with the well-known result for the single Ising chain.

From (15) and (12) we obtain the free energy for our system and therefore, the corresponding thermodynamic quantities, such as the internal energy and specific heat. Fig. 2 shows the energy in a zero field for several values of the interaction constants.

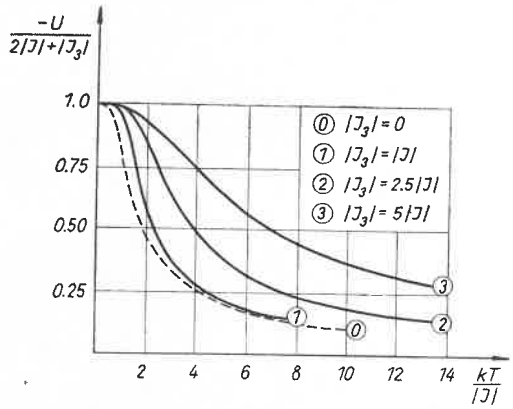

Fig. 2. Internal energy for $J_1 = J_2 = J$. The ordinate denote the normalized energy with respect to ground state, the dotted curve correspond to the energy of the single Ising chain

Fig. 3 shows the specific heat. The explicit expressions for the energy and specific heat are omitted here.

The high-temperature expansions for the partition function and internal energy U may be also obtained immediately and they are

$$\lambda_m(0) = 4\left(1+\frac{J_1^2+J_2^2+J_3^2}{2}\beta^2+\ldots\right) \tag{18}$$

$$U = -(J_1^2+J_2^2+J_3^2)\beta+\ldots \tag{19}$$

From (15) we may also obtain the leading term in the asymptotic expansion for $\lambda_m(0)$ when T tends to 0.

$$\lambda_m(0) \sim e^{\frac{|J_1|+|J_2|+|J_3|}{kT}}, \quad (J_1 J_2 > 0) \tag{20}$$

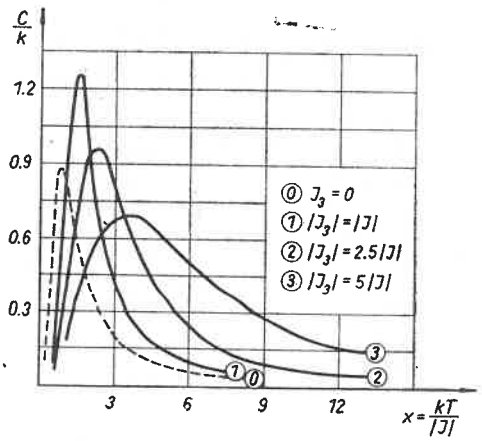

Fig. 3. Specific heat. The dotted curve correspond to 2 C/k for the single Ising chain

3. *The magnetization and the zero-field susceptibility*

A one-dimensional model with the finite-range interaction, such as the one used in this paper, should not exhibit phase transition. Let us recapitulate known arguments (see *e. g.* [6]) adopted for our case.

As we mentioned above, to each value of the field h corresponds a single root λ_m of the secular equation

$$\det(\mathscr{T} - \lambda \cdot I) \equiv g(l, \lambda) = 0 \tag{21}$$

where $g(l, \lambda)$ is an analytic function of the l, λ variables satysfying the condition

$$g_\lambda(l, \lambda_m) \neq 0. \tag{22}$$

According to the well-known theorem of analysis the equation (21) determines λ_m as the analytic function of the variable $l \equiv \beta h$. Consequently, f — the free energy in thermodynamical limit given by (12) is an analytic and, of course, even function of the external field for $T \neq 0$.

Introducing now the magnetization $m_{2N}(h)$ for the system consisting $2N$-spins

$$m_{2N}(h) = -\frac{\partial f_{2N}}{\partial h} \tag{23}$$

(we have $m_{2N}(0) = 0$, *i. e.* the finite system does not exhibit spontaneous magnetization) and the magnetization in the thermodynamical limit

$$m(h) = \lim_{N \to \infty} m_{2N}(h) \tag{24}$$

we obtain, after taking into account the statement d (see Introduction) and (12) that

$$m(h) = -\frac{\partial f}{\partial h}. \tag{25}$$

The immediate consequence of (25) is that $m(h)$ is a continuous and odd function of h. Hence, the spontaneous magnetization m_0 defined as

$$m_0 = \lim_{h \to 0+} m(h) \tag{26}$$

is equal to zero in the whole temperature range $(0, +\infty)$, as may be expected.

Now using the method, as in [4], we calculate the zero-field susceptibility κ_0

$$\kappa_0 = \frac{\partial m}{\partial h|_{h=0}}. \tag{27}$$

We have

$$\kappa_0 = -\frac{\partial^2 f}{\partial h^2|_{h=0}} = \frac{kT}{2\lambda_m} \frac{\partial^2 \lambda_m}{\partial h^2|_{h=0}} = -\frac{\beta}{2\lambda_m} \frac{g_{ll}(0, \lambda_m)}{g_\lambda(0, \lambda_m)}. \tag{28}$$

In our case

$$g(l, \lambda) = \lambda^4 + g_3(l)\lambda^3 + g_2(l)\lambda^2 + g_1(l)\lambda + g_0(l) \tag{29}$$

where

$$\begin{aligned} g_3(l) &= -2e^{u+v}(e^{-w} + \operatorname{ch} 2le^{w}), \\ g_2(l) &= 4[\operatorname{ch} 2l(e^{2u} \operatorname{sh} 2v + e^{2v} \operatorname{sh} 2u) + \operatorname{ch} 2w \operatorname{sh} 2(u+v)], \\ g_1(l) &= -8e^{u+v}(e^{-w} \operatorname{ch} 2l \operatorname{sh} 2u \operatorname{sh} 2v + e^{w} \operatorname{sh} 2u \operatorname{sh} 2v), \\ g_0(l) &= g_0(0) = 4(\operatorname{ch} 4u \operatorname{ch} 4v - \operatorname{ch} 4u - \operatorname{ch} 4v + 1). \end{aligned} \tag{30}$$

Thus, finally

$$\kappa_0 = -\frac{\beta}{2} \frac{g_{3,ll}(0)\lambda_m^2 + g_{2,ll}(0)\lambda_m + g_{1,ll}(0)}{4\lambda_m^3 + 3g_3(0)\lambda_m^2 + 2g_2(0) + g_1(0)} \tag{31}$$

where λ_m is given by (15). Numerical calculations of κ_0, which were based on this expression are presented here graphically (see Figs 4, 5, 6, 7).

From (31) we may obtain also the high and low-temperature expansions for κ_0. Thus, *e. g.*

$$kT\,\kappa_0 = 1 + (J_1 + J_2 + J_3)\,\beta + \ldots \tag{32}$$

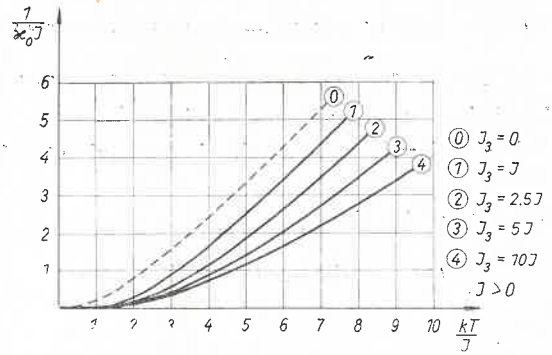

Fig. 4. Inverse susceptibility for ferromagnetic-ferromagnetic interaction ($J_1 = J_2 = J > 0$, $J_3 > 0$)

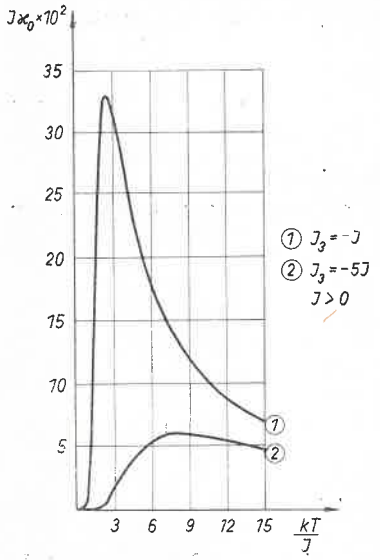

Fig. 5

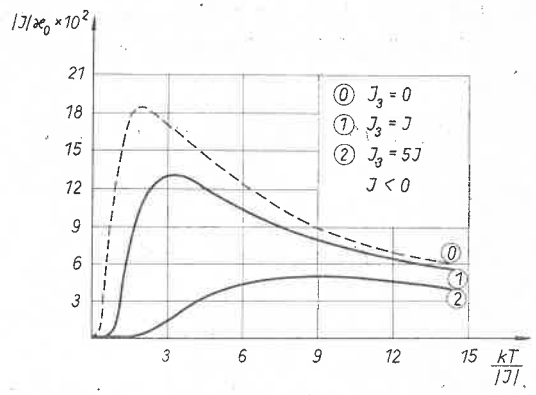

Fig. 6

Fig. 5. Susceptibility for ferromagnetic-antiferromagnetic interaction ($J_1 = J_2 = J > 0$, $J_3 < 0$)
Fig. 6. Susceptibility for antiferromagnetic-antiferromagnetic interaction ($J_1 = J_2 = J < 0$, $J_3 < 0$)

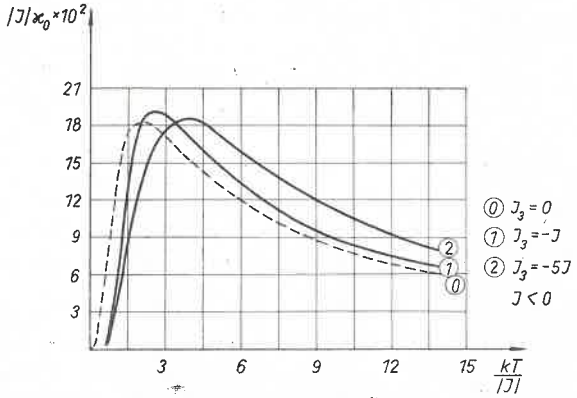

Fig. 7. Susceptibility for antiferromagnetic-ferromagnetic interaction ($J_1 = J_2 = J < 0$, $J_3 > 0$)

4. *The molecular field approximation (MFA)*

In this section we compare the exact solution with the solution given by MFA. In this approximation the chains are treated exactly with respect to the interaction of spins in each chain and the interaction between chains is approximated by the corresponding self-consistent field.

For this purpose, we take H_{2N} in the form:

$$H_{2N} = H_{2N}^{(0)}(\alpha_1, \alpha_2) + H_{2N}^{(1)}(\alpha_1, \alpha_2) \tag{33}$$

where

$$H_{2N}^{(0)} = J_3 N \alpha_1 \alpha_2 - (h + J_3 \alpha_2) \sum_{i=1}^{N} \sigma_i - (h + J_3 \alpha_1) \sum_{i=1}^{N} \mu_i - J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - J_2 \sum_{i=1}^{N} \mu_i \mu_{i+1}$$

$$H_{2N}^{(1)} = -J_3 \sum_{i=1}^{N} (\sigma_i - \alpha_1)(\mu_i - \alpha_2), \tag{34}$$

α_1 and α_2 are here the arbitrary parameters, to be determined later.

From Bogolubov's inequality (see, *e. g.*, [2]) we obtain (for the cyclic boundary conditions)

$$2f_{2N} \leqslant f_{2N}^{(u)} = J_3 \alpha_1 \alpha_2 + f_N^{(0)}(l, \alpha_2, u) + f_N^{(0)}(l, \alpha_1, v) - J_3(\alpha_1 - \langle \sigma \rangle_N)(\alpha_2 - \langle \mu \rangle_N), \tag{35}$$

where

$$f_N^{(0)}(l, \alpha, s) = -(N\beta)^{-1} \ln \sum_{\text{conf.}} \exp\left[(l + w\alpha) \sum_{i=1}^{N} t_i + s \sum_{i=1}^{N} t_i t_{i+1}\right],$$

$$(\alpha = \alpha_1, \alpha_2, \quad s = u, v, \quad t_i = \pm 1) \tag{36}$$

is the free energy per spin for the single Ising chain, on which the "field" $\tilde{h} = h + J_3 \alpha$ acts, and

$$\langle \sigma \rangle_N = -\frac{\partial f_N^{(0)}(l, \alpha_2, u)}{\partial h},$$

$$\langle \mu \rangle_N = -\frac{\partial f_N^{(0)}(l, \alpha_1, v)}{\partial h}. \tag{37}$$

The well-known solution for the single Ising chain (which may be easily obtained using the corresponding transfer matrix) gives

$$\lim_{N \to \infty} f_N^{(0)}(l, \alpha, s) = f^{(0)}(l, \alpha, s) = -\beta^{-1} \ln\left[e^s \operatorname{ch}(l + w\alpha) + \sqrt{e^{2s} \operatorname{ch}^2 (l + w\alpha) - 2 \operatorname{sh} 2s}\right] \tag{38}$$

where $f^{(0)}$ is the analytic function of the variable $l + w\alpha$. Hence we obtain that Bogolubov's inequality is also valid in the thermodynamical limit, *i. e.* the index N in (35) and (37) may be ommited.

The arbitrary hitherto parameters α_1, α_2 are now determined from the necessary condition for the minimum of $f^{(u)}(\alpha_1, \alpha_2)$

$$\frac{\partial f^{(u)}}{\partial \alpha_1} = 0, \qquad \frac{\partial f^{(u)}}{\partial \alpha_2} = 0. \tag{39}$$

Hence

$$\alpha_1^{(0)} = -\frac{1}{J_3}\frac{\partial f^{(0)}(l, \alpha_2^{(0)}, u)}{\partial \alpha_2} \equiv \sigma_0,$$

$$\alpha_2^{(0)} = -\frac{1}{J_3}\frac{\partial f^{(0)}(l, \alpha_1^{(0)}, v)}{\partial \alpha_1} \equiv \mu_0, \tag{40}$$

and

$$f^{u}(\alpha_1^{(0)}, \alpha_2^{(0)}) = J_3\sigma_0\mu_0 + f^{(0)}(l, \sigma_0, v) + f^{(0)}(l, \mu_0, u). \tag{41}$$

(Because of $\partial^2 f^{(0)}/\partial\alpha^2 > 0$, we see that $\frac{1}{2}f^{(u)}(\sigma_0, \mu_0)$ corresponds to the minimum of $\frac{1}{2}f^{(u)}$ if J_3 is sufficiently small.) $\frac{1}{2}f^{(u)}(\sigma_0, \mu_0)$ is now the upper bound for the exact free energy. Of course, $2f = f^{(u)}$ when $J_3 = 0$ (*i. e.* no interaction between chains).

The equations (40) are just the molecular field equations. When $h = 0$ their explicit form is

$$\sigma_0 = \frac{\operatorname{sh} w\mu_0}{\sqrt{\operatorname{sh}^2 w\mu_0 + e^{-4u}}}, \qquad \mu_0 = \frac{\operatorname{sh} w\sigma_0}{\sqrt{\operatorname{sh}^2 w\sigma_0 + e^{-4v}}}. \tag{42}$$

It is easy to interpret the equations (42) for ferromagnetic interaction when $J_1 = J_2 = J$ ($J > 0$, $J_3 > 0$). The right-hand sides of the system (42) are then the increasing and convex (upwards) functions of the variables $w\mu_0$ and $w\sigma_0$ respectively. Apart from the trivial solution $\sigma_0 = \mu_0 = 0$ the system (42) has then also the non-zero solution $\sigma_0(T) = \mu_0(T)$ in the interval $(0, T_c)$. The critical temperature T_c is determined by the equation

$$kT_c \ln\frac{kT_c}{J_3} = 2J. \tag{43}$$

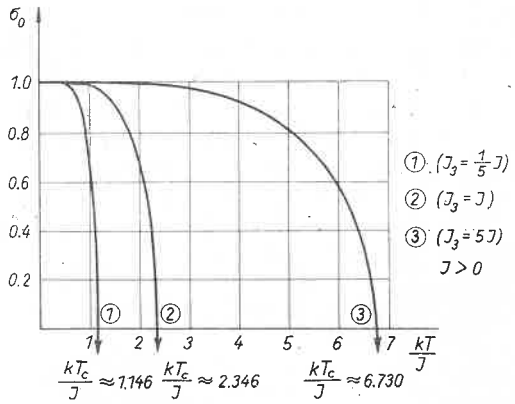

Fig. 8. Spontaneous magnetization of the double Ising chain in the molecular field approximation

The low-temperature expansion for the σ_0 has the form

$$\sigma_0 = 1-\tfrac{1}{2}e^{-4u-2w}+\ldots \tag{44}$$

The plots of σ_0 *vs* T are given in Fig. 8.

In conclusion, it shou'd be emphasized that the MFA — "intuitively obvious", especially for small J_3, gives quite wrong results compared with the exact solution, even in such a case as that considered above, when the system is divided into two macroscopic subsystems treated exactly and interacting *via* the self-consistent field.

In contrast to the upper bound estimation of f, we obtain a qualitatively correct result when we estimate its lower bound. From the known inequality for the matrix norms (see, *e. g.*, [7]), we have

$$\lambda_m(h) \leqslant [\sum_{i,j} \mathscr{T}_{ij}^2(h)]^{\frac{1}{2}}. \tag{45}$$

Hence

$$f(h) \geqslant f^{(l)}(h) \tag{46}$$

where

$$f^{(l)}(h) = -\frac{1}{4\beta} \ln \{8[\operatorname{ch} 2w \operatorname{ch} 2(u+v)+ \operatorname{ch} 2l \operatorname{ch} 2(u-v)]+(2 \operatorname{sh} 2le^{u+v+w})^2\} \tag{47}$$

and finally $\frac{\partial f_{(0)}^{(l)}}{\partial h} = 0$. The exact $f(h)$ becomes equal to its lower bound for $J_1 = J_2 = 0$, *i. e.* when the system consists of N statistically independent pairs of spins.

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