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Low-temperature asymptotics for the Ising model in an external magnetic field

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Abstract. The paper presents a method for calculating the low-temperature asymptotics of the free energy of the three-dimensional Ising model in an external magnetic field ($H \neq 0$). In this work an approach on the problem is employed, the main ideas of which were reported by the author earlier by an example of the two-dimensional Ising model in an external magnetic field. The results obtained are valid in the wide range of temperature and magnetic field values fulfilling the condition $[1 - \tanh^2(h/2)] \sim \varepsilon$, for $\varepsilon \ll 1$, where $h = \beta H$, β is the inverse temperature and H is the external magnetic field.

1. Formulation of the problem

As is well known, an exact solution for the two-dimensional (2D) Ising model in an external magnetic field ($H \neq 0$) has not yet been found. In the case of the three-dimensional (3D) Ising model an exact solution for a vanishing magnetic field does not exist ($H = 0$), to say nothing of the case of non-zero magnetic field. Despite the great successes in the investigation of Ising models made by means of the renormalization group method [2] and other approximate methods [1, 3–12] the problem of the calculation of various asymptotics for the 2D and 3D Ising models in the external magnetic field ($H \neq 0$) is still of great importance. In [1, 16] we calculated the low-temperature and high-temperature asymptotics for the 2D Ising model in an external magnetic field ($H \neq 0$), as well as the free energy for this model in the limit of an asymptotically vanishing magnetic field. In this paper we briefly discuss the calculation of the low-temperature asymptotics for the free energy in the 3D Ising model in an external magnetic field ($H \neq 0$), following the approach and the ideas we have introduced in [1].

Let us consider a cubic lattice built of N rows, M columns and K planes, to the vertices of which are assigned the numbers σ_{nmk} from the two-entry set ± 1. These quantities throughout this paper will be referred to as the Ising 'spins'. The multi-index (nmk) numbers vertices of the lattice, with n numbering rows, m numbering columns, and k numbering planes. The Ising model with nearest-neighbour interaction in an external magnetic field is described by the Hamiltonian of the form

$$\mathcal{H} = -\sum_{(n,m,k)=1}^{NMK} (J_1\sigma_{nmk}\sigma_{n+1,mk} + J_2\sigma_{nmk}\sigma_{n,m+1,k} + J_3\sigma_{nmk}\sigma_{nm,k+1} + H\sigma_{nmk}) \tag{1.1}$$

taking into account an anisotropy of the interaction between the nearest neighbours ($J_{1,2,3} > 0$), and the interaction of the spins σ_{nmk} with external magnetic field H, directed 'up' ($\sigma_{nmk} = +1$).

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The main problem consists of the calculation of the statistical sum for the system:

$$Z_3(h) = \sum_{\sigma_{111}=\pm 1} \cdots \sum_{\sigma_{NMK}=\pm 1} \mathrm{e}^{-\beta\mathcal{H}} = \sum_{\{\sigma_{nmk}=\pm 1\}} \exp\left[\sum_{nmk}(K_1\sigma_{nmk}\sigma_{n+1,mk} + K_2\sigma_{nmk}\sigma_{n,m+1,k} + K_3\sigma_{nmk}\sigma_{nm,k+1} + h\sigma_{nmk})\right] \tag{1.2}$$

where $K_{1,2,3} = \beta J_{1,2,3}$, $h = \beta H$, $\beta = 1/k_{\mathrm{B}}T$. Typical boundary conditions for the variables σ_{nmk} are the periodic ones. We take this standard assumption everywhere is the following. Let us note here that the statistical sum (1.2) is symmetric with respect to the change $(h \to -h)$.

In this paper we consider a limited version of the problem, that is the calculation of the low-temperature asymptotics for the free energy in the 3D Ising model in an external magnetic field. More precisely, if the coupling constants $(J_{1,2,3} = \text{const})$ and external magnetic field $(H = \text{const})$ are given, we consider the temperatures satisfying the condition $h \sim \varepsilon^{-1}$, $\varepsilon \ll 1$. To be more exact, we introduce a small parameter in the following way:

$$1 - \tanh^2(h/2) \sim \varepsilon \qquad \varepsilon \ll 1. \tag{1.3}$$

Then we consider the problem of the calculation of the free energy per one Ising spin in the thermodynamic limit, with an accuracy up to the order of $\sim\varepsilon^2$ in expansions of the operators associated with the spin interaction with an external magnetic field, as well as the interaction of spin with each other (details of the approximation used will be presented later). To the best of our knowledge, the problem formulated in this way has not been considered in existing literature and is of considerable importance.

2. Partition function

Let us consider an auxiliary 4D Ising model in an external magnetic field H on a simple 4D lattice $(N \times M \times K \times L)$. We write the Hamiltonian for the 4D Ising model with the nearest-neighbour interaction in the form

$$\mathcal{H} = -\sum_{n,m,k,l}(J_1\sigma_{nmkl}\sigma_{n+1,mkl} + J_2\sigma_{nmkl}\sigma_{n,m+1,kl} + J_3\sigma_{nmkl}\sigma_{nm,k+1,l} + J_4\sigma_{nmkl}\sigma_{nmk,l+1} + H\sigma_{nmkl}) \tag{2.1}$$

taking into account the anisotropy of the interaction between the nearest neighbours $(J_{1,2,3,4} > 0)$, and the interaction of the spins σ_{nmkl} with the external magnetic field H, directed 'up' $(\sigma_{nmkl} = +1)$. In equation (2.1) the multi-index $(nmkl)$ numbers the vertices of the 4D lattice, and the indices (n, m, k, l) take the values from 1 to (N, M, K, L), respectively. As in the case of the 3D Ising model, we introduce periodic boundary conditions for the variables σ_{nmkl}. Then we write the partition function $Z_4(h)$ in the form

$$Z_4(h) = \sum_{\sigma_{1111}=\pm 1} \cdots \sum_{\sigma_{NMKL}=\pm 1} \mathrm{e}^{-\beta\mathcal{H}} = \sum_{\{\sigma_{nmkl}=\pm 1\}} \exp\left[\sum_{nmkl}(K_1\sigma_{nmkl}\sigma_{n+1,mkl} + K_2\sigma_{nmkl}\sigma_{n,m+1,kl} + K_3\sigma_{nmkl}\sigma_{nm,k+1,l} + K_4\sigma_{nmkl}\sigma_{nmk,l+1} + h\sigma_{nmkl})\right] \tag{2.2}$$

where the quantities K_i and h are defined as for (1.2) [13, 14]. We can rewrite expression (2.2) using the well known method of the transfer matrix, in the form of a trace from the Lth power of the operator $\hat{T}$:

$$Z_4(h) = \mathrm{Tr}(\hat{T})^L \qquad \hat{T} = T_4 T_h^{1/2} T_3 T_2 T_1 T_h^{1/2} \tag{2.3}$$

where the operators $T_{1,2,3,4,h}$ are defined by the formulae

$$T_1 = \exp\left(K_1 \sum_{nmk} \tau^z_{nmk}\tau^z_{n+1,mk}\right) \qquad T_2 = \exp\left(K_2 \sum_{nmk} \tau^z_{nmk}\tau^z_{n,m+1,k}\right) \tag{2.4}$$

$$T_3 = \exp\left(K_3 \sum_{nmk} \tau^z_{nmk}\tau^z_{nm,k+1}\right) \qquad T_4 = (2\sinh 2K_4)^{NMK/2} \exp\left(K_4^* \sum_{nmk} \tau^x_{nmk}\right) \tag{2.5}$$

$$T_h = \exp\left(h \sum_{nmk} \tau^z_{nmk}\right) \tag{2.6}$$

and the quantities K_4 and K_4^* are coupled by the following relations:

$$\tanh(K_4) = \exp(-2K_4^*) \qquad \text{or} \qquad \sinh 2K_4 \sinh 2K_4^* = 1. \tag{2.7}$$

The Pauli spin matrices $\tau^{x,y,z}_{nmk}$ commute for $(nmk) \neq (n'm'k')$, and for given (nmk) these matrices satisfy the usual relations [17]. It is easy to see that the matrices $T_{1,2,3,h}$ commute with each other, but do not commute with the matrix T_4. If the quantities $K_i = 0$ $(i = 1, 2, 3)$, we immediately obtain the well known expressions describing the 3D Ising model on a simple cubic lattice. Namely, the transition to the 3D Ising model with respect to the coupling constants K_1, K_2 or K_3 is realized by taking $(K_1 = 0)$, $(K_2 = 0)$, or $(K_3 = 0)$, and removing the summation over n $(N = 1)$, m $(M = 1)$ or over k $(K = 1)$, respectively. As a result we obtain the standard expressions [13] for the 3D Ising model in an external magnetic field. In this process the operators T_i $(i = 1, 2, 3)$ in every one of the cases are identically equal to the unit operator $(T_i \equiv \hat{1})$. A slight different situation appears in the case of the transition to the 3D Ising model with respect to the coupling constant K_4. In this case we take $(K_4 = 0, L = 1)$, i.e. we remove the summation over l. As a consequence, we obtain the following expression for the operator T_4 from (2.5):

$$T_4^* \equiv T_4(K_4 = 0) = \prod_{nmk} (1 + \tau^x_{nmk}) \tag{2.8}$$

where we have used the relation (2.7). Then, after transition to the limit $(K_4 = 0, L = 1)$ in (2.3), we can write the following expression for the partition function for the 3D Ising model

$$Z_{3\mathrm{D}}(h) = \mathrm{Tr}(T_4^* T_h^{1/2} T_3 T_2 T_1 T_h^{1/2}) \tag{2.9}$$

where the matrices T_i are defined as in (2.4), (2.6) and (2.8). Now we go over to the fermionic representation. For this purpose one should write the matrices T_i in terms of the Pauli operators $\tau^{\pm}_{nmk}$ [14]

$$\tau^{\pm}_{nmk} = \tfrac{1}{2}(\tau^z_{nmk} \pm \mathrm{i}\tau^y_{nmk}) \tag{2.10}$$

which satisfy anticommutation relations for one vertex, and which commute for different vertices. Here, instead of Pauli operators

$$\tau'^{\pm}_{nmk} = \tfrac{1}{2}(\tau'^x_{nmk} \pm \mathrm{i}\tau'^y_{nmk})$$

we introduced, following [14] the new ones, $\tau^{\pm}_{nmk}$ by means of formulae (2.10). The point is that the transformations

$$\tau'^x \to \tau^z \qquad \tau'^y \to -\tau^y \qquad \tau'^z \to \tau^x$$

are the canonical transformations, which means that they are the same Pauli matrices which do no change the commutation relations. These transformations are introduced in order to have the exponents (2.4)–(2.6) containing only quadratic (T_{1234} operators in (2.6)) forms of Pauli operators $\tau^{\pm}_{nmk}$ but not the quaternary forms of these operators. As the next step one can move on from the representation by Pauli operators (2.10) to the representation by Fermi creation and annihilation operators [1]. It can be easily checked that for the 3D case the generalized Jordan–Wigner type transformations are of the form [16]

$$
\begin{aligned}
\tau^{+}_{nmk} &= \exp\left[\mathrm{i}\pi\left(\sum_{s=1}^{N}\sum_{p=1}^{M}\sum_{q=1}^{k-1}\alpha^{\dagger}_{spq}\alpha_{spq} + \sum_{s=1}^{N}\sum_{p=1}^{m-1}\alpha^{\dagger}_{spk}\alpha_{spk} + \sum_{s=1}^{n-1}\alpha^{\dagger}_{smk}\alpha_{smk}\right)\right]\alpha^{\dagger}_{nmk}\\
\tau^{+}_{nmk} &= \exp\left[\mathrm{i}\pi\left(\sum_{s=1}^{N}\sum_{p=1}^{M}\sum_{q=1}^{k-1}\beta^{\dagger}_{spq}\beta_{spq} + \sum_{s=1}^{n-1}\sum_{p=1}^{M}\beta^{\dagger}_{spk}\beta_{spk} + \sum_{p=1}^{m-1}\beta^{\dagger}_{npk}\beta_{npk}\right)\right]\beta^{\dagger}_{nmk}\\
\tau^{+}_{nmk} &= \exp\left[\mathrm{i}\pi\left(\sum_{s=1}^{N}\sum_{p=1}^{m-1}\sum_{q=1}^{K}\gamma^{\dagger}_{spq}\gamma_{spq} + \sum_{s=1}^{N}\sum_{q=1}^{k-1}\gamma^{\dagger}_{smq}\gamma_{smq} + \sum_{s=1}^{n-1}\gamma^{\dagger}_{smk}\gamma_{smk}\right)\right]\gamma^{\dagger}_{nmk}\\
\tau^{+}_{nmk} &= \exp\left[\mathrm{i}\pi\left(\sum_{s=1}^{N}\sum_{p=1}^{m-1}\sum_{q=1}^{K}\eta^{\dagger}_{spq}\eta_{spq} + \sum_{s=1}^{n-1}\sum_{q=1}^{K}\eta^{\dagger}_{smq}\eta_{smq} + \sum_{q=1}^{k-1}\eta^{\dagger}_{nmq}\eta_{nmq}\right)\right]\eta^{\dagger}_{nmk}\\
\tau^{+}_{nmk} &= \exp\left[\mathrm{i}\pi\left(\sum_{s=1}^{n-1}\sum_{p=1}^{M}\sum_{q=1}^{K}\omega^{\dagger}_{spq}\omega_{spq} + \sum_{p=1}^{M}\sum_{q=1}^{k-1}\omega^{\dagger}_{npq}\omega_{npq} + \sum_{p=1}^{m-1}\omega^{\dagger}_{npk}\omega_{npk}\right)\right]\omega^{\dagger}_{nmk}\\
\tau^{+}_{nmk} &= \exp\left[\mathrm{i}\pi\left(\sum_{s=1}^{n-1}\sum_{p=1}^{M}\sum_{q=1}^{K}\theta^{\dagger}_{spq}\theta_{spq} + \sum_{p=1}^{m-1}\sum_{q=1}^{K}\theta^{\dagger}_{npq}\theta_{npq} + \sum_{q=1}^{k-1}\theta^{\dagger}_{nmq}\theta_{nmq}\right)\right]\theta^{\dagger}_{nmk}
\end{aligned}
\tag{2.11}
$$

and analogously for the operators τ^{-}_{nmk} which are the Hermitian conjugations to (2.11). In [1] we obtained formulae for the relations between various Fermi operators and commutation relations for them for 2D case, which can be generalized to the 3D case. Indeed, the following relationships for the local occupation numbers are valid:

$$
\tau^{+}_{nmk}\tau^{-}_{nmk} = \alpha^{\dagger}_{nmk}\alpha_{nmk} = \beta^{\dagger}_{nmk}\beta_{nmk} = \gamma^{\dagger}_{nmk}\gamma_{nmk} = \eta^{\dagger}_{nmk}\eta_{nmk} = \omega^{\dagger}_{nmk}\omega_{nmk} = \theta^{\dagger}_{nmk}\theta_{nmk}. \tag{2.12}
$$

Then, applying the expressions (2.10)–(2.12) and considering results from [1], we can write the partition function (2.9) in the form

$$
Z_{3\mathrm{D}}(h) = (2\cosh^2 h/2)^{NMK}\langle 0|T^{*}|0\rangle = A\langle 0|U + \mu^2 CUD|0\rangle \qquad U \equiv T^{l}_{h}T_3T_2T_1T^{r}_{h} \tag{2.13}
$$

where $A = (2\cosh^2 h/2)^{NMK}$ and $\mu = \tanh(h/2)$, and the operators $T_{1,2,3}$, $T^{l,r}_{h}$ and C, D are of the form

$$
\begin{aligned}
T_1 &= \exp\left[K_1\sum_{n,m,k=1}^{N,M,K}(\alpha^{\dagger}_{nmk} - \alpha_{nmk})(\alpha^{\dagger}_{n+1,mk} + \alpha_{n+1,mk})\right]\\
T_2 &= \exp\left[K_2\sum_{n,m,k=1}^{N,M,K}(\beta^{\dagger}_{nmk} - \beta_{nmk})(\beta^{\dagger}_{n,m+1,k} + \beta_{n,m+1,k})\right]\\
T_3 &= \exp\left[K_3\sum_{n,m,k=1}^{N,M,K}(\theta^{\dagger}_{nmk} - \theta_{nmk})(\theta^{\dagger}_{nm,k+1} + \theta_{nm,k+1})\right]
\end{aligned}
\tag{2.14}
$$

and

$$
\begin{aligned}
T^{r}_{h} &= \exp\left\{\mu^2\left[\sum_{nmk}\sum_{s=1}^{N-n}\alpha^{\dagger}_{nmk}\alpha^{\dagger}_{n+s,mk} + \sum_{nn'mk}\sum_{t=1}^{M-m}\alpha^{\dagger}_{nmk}\alpha^{\dagger}_{n',m+t,k} + \sum_{nn'mm'k}\sum_{l=1}^{K-k}\alpha^{\dagger}_{nmk}\alpha^{\dagger}_{n'm',k+l}\right]\right\}\\
T^{l}_{h} &= \exp\left\{\mu^2\left[\sum_{nmk}\sum_{l=1}^{K-k}\theta_{nm,k+l}\theta_{nmk} + \sum_{nmkk'}\sum_{t=1}^{M-m}\theta_{n,m+t,k}\theta_{nmk'} + \sum_{nmm'kk'}\sum_{s=1}^{N-n}\theta_{n+s,mk}\theta_{nm'k'}\right]\right\}
\end{aligned}
\tag{2.15}
$$

$$
C = \sum_{nmk}\theta_{nmk} \qquad D = \sum_{nmk}\alpha^{\dagger}_{nmk}.
$$

Here and below $\sum_{n,m,\ldots}$ means summation over the complete set of indices ($n = 1, \ldots, N$; $m = 1, \ldots, M$; etc). It is obvious that the operator $\hat{G}$

$$\hat{G} = (-1)^{\hat{S}} \qquad \hat{S} = \sum_{nmk} \alpha^{\dagger}_{nmk}\alpha_{nmk} \tag{2.16}$$

where $\hat{S}$ is the operator of the total number of particles, commutes with the operator T^*, (2.13). Therefore, we can divide all states of the operator T^* into states with an even ($\lambda_{\hat{G}} = +1$) or odd number of particles ($\lambda_{\hat{G}} = -1$) with respect to the operator $\hat{G}$, (2.16). The form of the operators $T_{1,2,3}$ does not change under such transformation, only the boundary conditions for the operators ($\alpha_{nmk}, \ldots$) do. In the case of even states ($\lambda_{\hat{G}} = +1$), antiperiodic boundary conditions are chosen and in the case of odd states, periodic ones are chosen [1].

The next step is the transition to the momentum representation:

$$\alpha^{\dagger}_{nmk} = \frac{\exp(\mathrm{i}\pi/4)}{(NMK)^{1/2}} \sum_{qp\nu} \mathrm{e}^{-\mathrm{i}(nq+mp+k\nu)}\xi^{\dagger}_{qp\nu} \qquad \beta^{\dagger}_{nmk} \to \eta^{\dagger}_{qp\nu} \qquad \theta^{\dagger}_{nmk} \to \zeta^{\dagger}_{qp\nu}.$$

Here we have introduced, in terms of the occupation numbers for fixed $(qp\nu)$, the corresponding ξ-, η- and ζ-Fermi creation and annihilation operators in the finite-dimensional Fock space of $2^8 = 256$ dimensions. Then, after a series of transformations and calculations we arrive at the following formula for the partition function (2.13):

$$Z^{+}_{3\mathrm{D}}(h) = A\left(\prod_{0<q,p,\nu<\pi} A_1^4(q)\right)\left(\prod_{0<q,p,\nu<\pi} A_3^4(\nu)\right)\langle 0|T_3^*(h)T_2T_1^*(h)|0\rangle \tag{2.17}$$

where the operators $T_1^*(h)$, T_2 and $T_3^*(h)$ are of the form

$$\begin{aligned}
T_1^*(h) &= \exp\left[\sum_{0<q,p,\nu<\pi} B_1(q)(\xi^{\dagger}_{-q-p-\nu}\xi^{\dagger}_{qp\nu} + \xi^{\dagger}_{-q-p\nu}\xi^{\dagger}_{qp-\nu} + \xi^{\dagger}_{-qp-\nu}\xi^{\dagger}_{q-p\nu} + \xi^{\dagger}_{-qp\nu}\xi^{\dagger}_{q-p-\nu})\right] \\
T_2 &= \exp\left\{2K_2 \sum_{0<q,p,\nu<\pi} [\cos p(\eta^{\dagger}_{qp\nu}\eta_{qp\nu} + \cdots) + \sin p(\eta^{\dagger}_{-q-p-\nu}\eta^{\dagger}_{qp\nu} + \cdots\right. \\
&\qquad \left. + \eta_{qp\nu}\eta_{-q-p-\nu} + \cdots]\right\} \\
T_3^*(h) &= \exp\left[\sum_{0<q,p,\nu<\pi} B_3(\nu)(\zeta_{qp\nu}\zeta_{-q-p-\nu} + \zeta_{-qp\nu}\zeta_{q-p-\nu} + \zeta_{q-p\nu}\zeta_{-qp-\nu}\right. \\
&\qquad \left. + \zeta_{-q-p\nu}\zeta_{qp-\nu})\right]
\end{aligned} \tag{2.18}$$

and $A_1(q,h), \ldots$ are defined by the expressions

$$\begin{aligned}
A_1(q,h) &= \cosh 2K_1 - \sinh 2K_1 \cos q + \alpha(h,q)\sinh 2K_1 \sin q \\
A_3(\nu,h) &= \cosh 2K_3 - \sinh 2K_3 \cos \nu + \alpha(h,\nu)\sinh 2K_3 \sin \nu \\
B_1(q,h) &= \frac{\alpha(h,q)[\cosh 2K_1 + \sinh 2K_1 \cos q] + \sinh 2K_1 \sin q}{A_1(q,h)} \\
B_3(\nu,h) &= \frac{\alpha(h,\nu)[\cosh 2K_3 + \sinh 2K_3 \cos \nu] + \sinh 2K_3 \sin \nu}{A_3(\nu,h)} \\
\alpha(h,q) &= \tanh^2(h/2)\frac{1+\cos q}{\sin q} \qquad \alpha(h,\nu) = \tanh^2(h/2)\frac{1+\cos \nu}{\sin \nu}.
\end{aligned} \tag{2.19}$$

In the formula for $Z^{+}_{3\mathrm{D}}(h)$ the (+) sign means that we consider the case of even states ($\lambda_{\hat{G}} = +1$) with respect to the operator $\hat{G}$, (2.16). It is obvious that for $h = 0$ we have the 3D Ising model for a vanishing magnetic field. Then, for $K_1 = 0$ ($K_2 = 0$ or $K_3 = 0$) the expression (2.17) for the statistical sum describes the 2D Ising model in an external magnetic field [1].

3. Solution

Let us consider the calculation of the free energy per one Ising spin in an external magnetic field in the approximation described briefly in the introduction. For this aim, let us consider the operators $T_1^*(h)$ and $T_3^*(h)$ in the 'coordinate' representation

$$T_1^*(h) = \exp\left[\sum_{nmk}\sum_{s=1}^{N-n} a(s)\alpha_{nmk}^{\dagger}\alpha_{n+s,mk}^{\dagger}\right]$$
$$T_3^*(h) = \exp\left[\sum_{nmk}\sum_{l=1}^{K-k} c(l)\theta_{nm,k+l}\theta_{nmk}\right] \tag{3.1}$$

where the 'weights' $a(s)$ and $c(l)$ are defined by the formulae

$$a(s) = \frac{1}{N}\sum_{0<q<\pi} 2B_1(q)\sin(sq) = z_1^{*s} + \tanh^2 h_1^* \frac{1 - z_1^{*s}}{(1 - z_1^*)^2} \qquad s = 1, 2, 3, \ldots$$
$$c(l) = \frac{1}{K}\sum_{0<\nu<\pi} 2B_3(\nu)\sin(l\nu) = z_3^{*l} + \tanh^2 h_3^* \frac{1 - z_3^{*l}}{(1 - z_3^*)^2} \qquad l = 1, 2, 3, \ldots. \tag{3.2}$$

We have introduced renormalized quantities $(K_{1,3}^*, h_{1,3}^*)$ which defined as follows:

$$\sinh 2K_{1,3}^* = \beta_{1,3}[\sinh 2K_{1,3}(1 - \tanh^2(h/2)]$$
$$\cosh(2K_{1,3}^*) = \beta_{1,3}[\cosh 2K_{1,3} + \tanh^2(h/2)\sinh 2K_{1,3}]$$
$$\beta_{1,3} = [1 + 2\tanh^2(h/2)\sinh 2K_{1,3}\exp(2K_{1,3})]^{-1/2}$$
$$\tanh^2 h_{1,3}^* = \tanh^2(h/2)\frac{\beta_{1,3}\exp(2K_{1,3})}{\cosh^2 K_{1,3}^*}. \tag{3.3}$$

These formulae are valid for $(K_{1,3} \geqslant 0)$. As in the case of the 2D Ising model [1, 18], in this case one can also introduce a diagrammatic representation for the vacuum matrix element $S \equiv \langle 0|T_3^*(h)T_2T_1^*(h)|0\rangle$. The diagrammatic representation for the vacuum matrix element $S \equiv \langle 0|T_3^*(h)T_2T_1^*(h)|0\rangle$ is reduced to the calculation of the generating function for the Hamiltonian graphs on the simple cubic $(N \times M \times K)$ lattice which is by no means a trivial problem. Computation of the vacuum matrix element S, which enters the formula (2.17) for $Z_{3D}^+(h)$ in the general case, where the 'weights' (3.2) are arbitrary is, at least at present, impossible. Nevertheless, there exists a special case in which we can calculate the quantity S in the 3D case. Namely, this is the case where the 'weights' (3.2) are independent of l and s. In this case one should put the parameters $K_{1,3}$ equal to zero ($K_{1,3} = 0$) in formula (2.13), and then express the operators $T_h^{l,r}$ in terms of the Fermi β-operators (2.11) of creation and annihilation, having in mind the calculation of S. After transition to the momentum representation, one should calculate the vacuum matrix element $S^*(y_1, y_3, z_2)$

$$S^*(y_1, y_3, z_2) \equiv \langle 0|T^l(y_3)T_2T^r(y_1)|0\rangle \qquad y_{1,3} \equiv \tanh^2 h_{1,3}$$

where $z_2 = \tanh K_2$, so the calculation of $S^*(y_1, y_3, z_2)$ becomes trivial. (Here we have introduced the following change of notation: $h/2 \to h_1$ for the operator T_h^r and $h/2 \to h_3$ for the operator T_h^l.) The result of the calculations for $S^*(y_1, y_3, z_2)$ can be written down as:

$$S^*(y_1, y_3, z_2) = (2\cosh^2 K_2)^{NMK/2}\prod_{0<qp\nu<\pi}[(1 - 2z_2\cos p + z_2^2)(1 - \cos p)$$
$$+2z_2(y_1 + y_3)\sin^2 p + y_1y_3(1 + 2z_2\cos p + z_2^2)(1 + \cos p)]^4. \tag{3.4}$$

It can be shown that the expression

$$-\beta F(h) = \lim_{NMK\to\infty} \frac{1}{NMK} \ln\Bigg[(2\cosh^2 h/2)^{NMK} \Bigg(\prod_{0<qp\nu<\pi} A_1^4(q)\Bigg)\Bigg(\prod_{0<qp\nu<\pi} A_3^4(\nu)\Bigg) \times S^*(y_1, z_2, y_3)\Bigg]$$

describing, at $K_{1,3} = 0$, $y_1 = y_3 = \tanh^2 h/2$, the free energy for the 1D Ising model in the thermodynamic limit, is reduced exactly to the classic Ising result.

This result (3.4) can be used further to calculate the free energy in the approximation discussed above (1.3). For this aim, let us note that the condition $[\tanh^2 h^*_{1,3}/(1 - z^*_{1,3})^2] \to 1$ are equivalent, accordingly to (3.3), to the condition $(\exp(-2K_{1,3})(1 - \tanh^2 h/2) \to 0)$. It follows from this equation that for fixed ($J_{1,3} = \text{const}$, $H = \text{const}$) these conditions are satisfied for such temperatures T, when $(h/2) \sim \varepsilon^{-1}$, $\varepsilon \ll 1$. In this case we can use the result (3.4). Namely, let us consider the formulae (2.19) for $B_{1,3}$, written in terms of the renormalized parameters $(h^*_{1,3}, K^*_{1,3})$:

$$B_{1,3} = \frac{\tanh^2 h^*_{1,3}(\sin q(\nu)/[1 - \cos q(\nu))] + 2z^*_{1,3} \sin q(\nu)}{1 - 2z^*_{1,3}\cos q(\nu) + {z^*_{1,3}}^2} \tag{3.5}$$

where $z^*_{1,3} = \tanh K^*_{1,3}$. Next, since the following equalities are satisfied,

$$\frac{z^*_{1,3}}{1 + {z^*_{1,3}}^2} = \frac{z_{1,3}(1 - \tanh^2 h/2)}{1 + 2z_{1,3}\tanh^2 h/2 + z^2_{1,3}}$$

then, if we introduce a small parameter $[1 - \tanh(h/2)] \sim \varepsilon$ ($\varepsilon \ll 1$) and expand $B_{1,3}$ into a power series in ε ($z^*_{1,3} \sim \varepsilon$), we obtain

$$B_{1,3} = \frac{(\tanh^2 h^*_{1,3} + 2z^*_{1,3})\sin q(\nu)}{1 - \cos q(\nu)} + \sim\varepsilon^2.$$

This formula gives the following expressions for the 'weights' $a(s)$ and $c(l)$ from (3.2) in this approximation

$$a(s) = \tanh^2 h^*_1 + 2z^*_1 \qquad c(l) = \tanh^2 h^*_3 + 2z^*_3 \tag{3.6}$$

with the accuracy to the small parameter $\sim\varepsilon^2$. As a result in this approximation the 'weights' $a(s)$ and $c(l)$ do not depend on (s, l). Finally, if we substitute into the expression (3.4) for $S^*(y_1, y_3, z_2)$ the parameters $y_1 \to a(s)$ and $y_3 \to c(l)$ from (3.6), we have the following formula for the free energy per one Ising spin $F_{3D}(h)$ in the thermodynamic limit:

$$\begin{aligned}-\beta F_{3D}(h) \sim{}& \ln(2^{3/2}\cosh K^*_1 \cosh K_2 \cosh K^*_3 \cosh^2 h/2) + \frac{1}{2\pi}\int_0^\pi \ln[(1 - 2z_2\cos p + z_2^2)\\ &\times(1 - \cos p) + 2z_2(\tanh^2 h^*_1 + \tanh^2 h^*_3 + 2z^*_1 + 2z^*_3)\sin^2 p + (\tanh^2 h^*_1 + 2z^*_1)\\ &\times(\tanh^2 h^*_3 + 2z^*_3)(1 + 2z_2\cos p + z_2^2)(1 + \cos p)]\,\mathrm{d}p\end{aligned} \tag{3.7}$$

where $\beta = 1/k_B T$, $z_2 = \tanh K_2$ and $h^*_{1,3}$ and $K^*_{1,3}$ are coupled with h and $K_{1,3}$ by the relations (3.3). One can show that, as it was done for the 1D and 2D Ising models [1], in the case of the odd states ($\lambda_{\hat{G}} = -1$) with respect to the operator $\hat{G}$, (2.16), the formula for $F_{3D}(h)$ is described in the thermodynamic limit by (3.7). Let us note that the asymptotics (3.7) obtained above can also be applied in the case of rather strong magnetic fields (H), as far as the condition $(1 - \tanh h) \sim \varepsilon$, $\varepsilon \ll 1$, $(T = \text{const})$ is satisfied.

It is well known that there are a great number of publications (see, for example, the series in many volumes *Phase Transitions and Critical Phenomena* ed C Domb and M S Green) related, in some way or other, to low- and high-temperature expansions for the Ising model in a zero, as well as in a non-zero, external magnetic field (see, for example, [6–9]). It should be noted that the form of these expansions is not practically suitable for the calculations and phase diagram constructions, which can be seen from the continuous attempts to search for new approaches to the solution of the problem (see, for example, [10–12]). From this point of view, our result (3.7) is just another attempt of that kind. As it follows from the derivation procedure, the validity range in the field H and temperature T of expansion (3.7) is large enough. In other words, the boundaries of this validity range are 'floating' and this effect makes our result different from the others.

4. Final remarks

The main result given by formula (3.7) can be applied, in the setting of equilibrium thermodynamics, to the analysis of the 3D Ising magnetic, lattice gas and to the 3D models of binary alloys [19, 20] under the conditions for the temperature and magnetic field given by (1.3). Such analyses, as well as the construction of appropriate phase diagrams for the models mentioned above is, in our opinion, of great interest. They deserve to be considered in a separate publication.

Here we also make some important remarks. The preliminary numerical analysis of the solution (3.7) and its comparison with the results for the 3D Ising model in the external field obtained previously by other authors (see, for example, [6, 8]) demonstrate the good agreement between the results for the common domain of the parameters $(K_{1,2,3}, h)$ accurate up to an accepted approximation. However, the (3.7) solution is of some specific character, since the applicability of (3.7) depends on the external magnetic field H and can approach the temperature $T \geqslant T_c$. The point is that in deriving (3.7) we actually summed up the infinite series taking into account the main terms for the given values of the parameters (H, T). Therefore, we should expect that (3.7) would be suitable for the models of lattice gases and binary alloys [17, 19, 20]. On the other hand, comparison of solution (3.7) with recent results obtained for the Ising model in an external magnetic field (see, for example, [22] and the references therein) is confronted with serious difficulties and further investigations are required. These difficulties arise from the fact that these results look as if they are fragmentary by character, because as a rule they are the by-product of investigations of other statistical mechanics and lattice quantum field theory models. For this reason, very often it is difficult to determine the field of application of the results obtained and to perform any comparison between them. A review of the great number of works devoted to the numerical simulation of the Ising model in an external field is also beyond the scope of this paper; this will be done elsewhere.

The other important feature of the method presented here is the possibility of deriving the expressions for the free energy of the 3D Ising model in the limiting case of the magnetic field tending to zero $(H \to 0, N, M, K \to \infty)$, if we know the exact solution for the 3D Ising model in a zero external magnetic field $(H = 0)$. This possibility results from equations (3.2) and (3.3) describing the renormalized interaction constants $K^*_{1,3}$ and corresponds, as was shown in [1], to the results obtained by Yang [21] for the 2D Ising model. In conclusion, it is worth mentioning that as far as our ideas of introducing the Hamiltonian graphs into this field of theoretical physics is concerned, they have already been taken up by others (see, for example, [23]).

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