ON THE TWO- AND THREE-DIMENSIONAL ISING–ONSAGER PROBLEM IN PRESENCE OF MAGNETIC FIELD*

M.S. Kochmański

Institute of Physics, Pedagogical University
T.Rejtana 16 A, 35–310 Rzeszów, Poland
e-mail:wsprze@atos.warman.com.pl

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In this paper a new approach to solving the Ising–Onsager problem in external magnetic field is investigated. The expression for free energy per Ising spin in external field both for the two dimensional and three dimensional Ising model with interaction of the nearest neighbors are derived. The representations of free energy being expressed by multidimensional integrals of Gauss type with the appropriate dimensionality are shown. The possibility of calculating the integrals and the critical indices on the base of the derived representations for free energy is investigated.

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1. Introduction

It is well known that the Ising–Onsager problem [1, 2] in an external magnetic field has not been solved , despite intensive efforts of a few generations of physicists and mathematicians. By the problem we mean the exact calculation of the statistical sum for the Ising model with interaction of the nearest neighbors both in the two dimensional case (in finite external field) and in the three dimensional case (in external field as well as without such a field). Therefore, we do not intend to present a variety of approximate methods and approaches to solving the Ising–Onsager problem. Detailed discussion of these matters could be found in numerous well known papers and monographs. We note here only the paper by Yang [3], where the problem was investigated for the case of infinitely small external field in two dimensions. In our opinion, the efforts to find an exact solution to the Ising–Onsager problem is of great interest. The reason is, the Ising

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models are connected with numerous other models of statistical mechanics and quantum field theory [4–7]. Therefore the present paper is treated as the next step in the direction described above.

2. The partition function

Here we consider firstly the two dimensional case($d = 2, H \neq 0$), and then we will report on the results for the three dimensional case ($d = 3, H \neq 0$) without going into details of the derivations. Let us consider a rectangular lattice consisting of M columns and N lines, in nodes of which are given variables σ_{nm} which take values ± 1.

These variables will be called "spins". The collective index nm number nodes of the lattice; n number of line, m numbers of column. The Ising model with the nearest neighbors interaction is given by the following form of the Hamiltonian:

$$\mathcal{H} = -J_2 \sum_{nm} \sigma_{nm}\sigma_{n+1,m} - J_1 \sum_{nm} \sigma_{nm}\sigma_{n,m+1} - H \sum_{nm} \sigma_{nm}, \tag{2.1}$$

which takes into account the possible anisotropy of the interaction between the nearest neighbors and also interaction of spins σ_{nm} with external field H, which is directed "upwards" ($\sigma_{nm} = +1$). The investigated problem consists of calculation of the statistical sum for the system:

$$\begin{aligned} Z(h) &= \sum_{\sigma_{11}=\pm 1} \cdots \sum_{\sigma_{NM}=\pm 1} \exp\left(-\beta \mathcal{H}\right) \\ &= \sum_{(\sigma_{nm}=\pm 1)} \exp\left[\sum_{n,m=1}^{NM} \left(K_2 \sigma_{nm}\sigma_{n+1,m} + K_1 \sigma_{nm}\sigma_{n,m+1} + h\sigma_{nm}\right)\right], \end{aligned} \tag{2.2}$$

where

$$K_{1,2} = \beta J_{1,2}, \qquad h = \beta H, \qquad \beta = 1/k_B T. \tag{2.3}$$

Typically, periodic boundary conditions on variables σ_{nm} are imposed and we will assume this everywhere below. Let us note that the statistical sum (2.2) is symmetric with respect to the change $h \to -h$.

As is known [8], the statistical sum (2.2) can be represented in the form of the trace of the T-operator (*T-transfer matrix*):

$$Z(h) = \operatorname{Tr}(T)^M = \operatorname{Tr}\left[(2\sinh 2K_1)^{(N/2)} T_1 T_2 T_h\right]^M, \tag{2.4}$$

where the matrices $T_{1,2,h}$ are of the form:

$$T_1 = \exp\left(K_1^* \sum_{n=1}^{N} \sigma_n^x\right), \tag{2.5}$$

$$T_2 = \exp\left(K_2 \sum_{n=1}^{N} \sigma_n^z \sigma_{n+1}^z\right), \qquad \sigma_{N+1}^z = \sigma_1^z, \tag{2.6}$$

$$T_h = \exp\left(h \sum_{n=1}^{N} \sigma_n^z\right), \tag{2.7}$$

and K_1^* and K_1 are connected by the relations:

$$\exp(-2K_1) = \tanh(K_1^*), \quad \textit{or} \quad \sinh(2K_1)\sinh(2K_1^*) = 1. \tag{2.8}$$

In the formulae (2.5)–(2.7) the quantities $(\sigma_n^{x,y,z})$, $(n = 1, 2, ...N)$ are well known from quantum mechanics 2^N-dimensional matrices:

$$\sigma_n^{x,y,z} = 1 \otimes 1 \otimes ... \otimes \sigma^{x,y,z} \otimes ... \otimes 1, \quad (N \text{ factors}),$$

where $\sigma^{x,y,z}$ — two dimensional spin Pauli matrices:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.9}$$

satisfying the standard transposition relations:

$$(\sigma^k)^2 = 1, \quad \sigma^k\sigma^j + \sigma^j\sigma^k = 0, \quad (k, j) = x, y, z; \ ; \sigma^x\sigma^y = i\sigma^z, \ ... \tag{2.10}$$

For example, spin matrices for the n-th electron in the system consisting of N nonrelativistic electrons are exactly the matrices $\sigma_n^{x,y,z}$. It is known that for $n \neq n'$ spin matrices $\sigma_n^{x,y,z}$ commute and for any given particular n they formally satisfy relations (2.10). It follows from this that matrices T_2 and T_h, (2.6)–(2.7) commute but they do not commute with the matrix T_1, (2.5), *i.e.*

$$[T_2, T_h]_- = 0, \quad [T_h, T_1]_- \neq 0, \quad [T_2, T_1]_- \neq 0. \tag{2.11}$$

It follows from (2.11) that under Tr (...) we can write for the statistical sum (2.4) the expression:

$$Z(h) = \mathrm{Tr}\,(\gamma T_1 T_h^{1/2} T_2 T_h^{1/2})^M = \mathrm{Tr}\,(\gamma T_h^{1/2} T_1 T_h^{1/2} T_2)^M \equiv \mathrm{Tr}\,(P)^M, \tag{2.12}$$

$$P \equiv (2\sinh 2K_1)^{N/2} T_h^{1/2} T_1 T_h^{1/2} T_2, \tag{2.13}$$

where we used the identity $\mathrm{Tr}\,(AB) \equiv \mathrm{Tr}\,(BA)$.

Now we will consider in details the matrix $U \equiv T_h^{1/2} T_1 T_h^{1/2}$; since the matrices σ_n^x and $\sigma_{n'}^z$, commute for $n \neq n'$, we can write the matrix U in the form:

$$U \equiv T_h^{1/2} T_1 T_h^{1/2} = \prod_{n=1}^{N} e^{(h/2)\sigma_n^z} e^{K_1^* \sigma_n^x} e^{(h/2)\sigma_n^z} \equiv \prod_{n=1}^{N} U_n. \tag{2.14}$$

Further the matrix U_n can be represented in the following form:

$$\begin{aligned} U_n &= e^{(h/2)\sigma_n^z}(\cosh K_1^* + \sigma_n^x \sinh K_1^*)e^{(h/2)\sigma_n^z} \\ &= \exp\left[\omega\left(\frac{\cosh K_1^* \sinh h}{\sinh\omega}\sigma_n^z + \frac{\sinh K_1^*}{\sinh\omega}\sigma_n^x\right)\right], \end{aligned} \tag{2.15}$$

where ω is a positive root of the equation:

$$\cosh\omega = \cosh K_1^* \cosh h, \tag{2.16}$$

In determination of the expression (2.15) we used the identity:

$$\exp(\mu t) = \cosh\mu + t\sinh\mu, \quad t^2 = 1. \tag{2.17}$$

It is easy to see that for $h = 0$ we obtain from (2.12) the standard expression for the statistical sum Z for the two dimensional Ising model without external field [5, 6].

2.1. The 1D Ising model

One can relatively easily show that (2.12) becomes:

$$Z(h) = \mathrm{Tr}\left[(2\sinh 2K_1)^{N/2}\prod_{n=1}^{N} U_n T_2\right]^M, \tag{2.18}$$

where U_n is given by the formula (2.15), and it describes correctly the transition to the one dimensional Ising model both in the constant K_1, and in the constant K_2. Indeed, if we take $K_2 = 0$ and $N = 1$, what corresponds to neglecting summation over n we obtain:

$$Z_1(h) = \mathrm{Tr}\left[(2\sinh 2K_1)^{1/2}U_0\right]^M, \tag{2.19}$$

where the matrix U_0 is given by (2.15), where the index n was omitted. Eigenvalues of the matrix U_0 can be easily obtained:

$$\lambda^{\pm} = \exp(\pm\omega),$$

where ω is the positive root for the equation (2.16). As a result we obtain the following formula describing free energy per spin in the thermodynamic limit:

$$\begin{aligned} f(h) &= -\frac{1}{\beta}\lim_{M\to\infty}\frac{1}{M}\ln Z_1(h) \\ &= -\frac{1}{\beta}\ln\left[e^{K_1}\cosh h + (e^{2K_1}\sinh^2 h + e^{-2K_1})^{1/2}\right], \end{aligned} \tag{2.20}$$

i.e. the known classical expression [1].

Transition to the onedimensional Ising model limit in the constant K_1 could be done by taking $K_1 \to 0$, and $M = 1$, *i.e.* we neglect summation over the index m and go to the limit $K_1 \to 0$. As a result we obtain from (2.18):

$$Z_1(h) = \mathrm{Tr}\left[\prod_{n=1}^{N}(1+\sigma_n^x)T_2T_h\right], \tag{2.21}$$

where we used the transition to the limit:

$$\lim_{K_1\to 0}(2\sinh 2K_1)^{1/2}\exp(K_1^*\sigma_n^x) = (1+\sigma_n^x),$$

where we took into account the relation (2.8) between K_1 and K_1^*. Note here that the factors $(1+\sigma_n^x)$, entering the expression (2.21), are simply necessary to get the correct result. To calculate the trace (2.21), it is convenient to apply the fermion representation [6, 8]. Omitting some calculations we can write for (2.21) in the form:

$$Z_1(h) = \mathrm{Tr}\,(DT_2^{\pm}T_h), \tag{2.22}$$

where the operators D, $T_2^{\pm}$ and T_h, expressed in terms of Fermi creation and annihilation operators (c_n^+, c_n) are of the form:

$$D = \prod_{n=1}^{N}\left[1+(-1)^{c_n^+c_n}\right]. \tag{2.23}$$

$$T_2^{\pm} = \exp\left[K_2\sum_{n=1}^{N}(c_n^+ - c_n)(c_{n+1}^+ + c_{n+1})\right], \tag{2.24}$$

$$T_h = \exp\left\{h\sum_{n=1}^{N}\exp\left[i\pi\sum_{p=1}^{n-1}c_p^+c_p\right](c_n^+ + c_n)\right\}, \tag{2.25}$$

In the formula (2.24) the sign (+) is related to states that are even with respect to the operator of the complete number of particles ($\hat{N} = \sum_{n=1}^{N} c_n^+c_n$) and to which correspond anticyclic boundary conditions, while the sign (−) to the odd states, to which correspond cyclic boundary conditions. It is easy to see that because of the multiplicative character of the operator D, (2.23), all diagonal matrix elements in (2.22) vanish with the exception of the vacuum-vacuum matrix element, *i.e.*:

$$Z_1(h) = 2^N\langle 0 \mid (T_2^{\pm}T_h) \mid 0\rangle, \tag{2.26}$$

where the operators $T_2^{\pm}$ and T_h are defined by (2.24)–(2.25). Then, "acting" with the operator T_h on the vacuum state $\mid 0 >$, and using the Hausdorff–Baker formula [10], $(\alpha, \beta = const)$:

$$\exp(\alpha x)\exp(\beta y) = \exp(\alpha x + \beta y + (\alpha\beta/2)[x,y]_-)\,,$$

$$[x,z]_- = [y,z]_- = 0, \qquad z \equiv [x,y]_-\,,$$

the operator T_h, (2.25) can be reduced to the "effective" form (in the sense of action on $\mid 0 >$):

$$T_h = \cosh^N(h)\exp\left[\tanh^2 h \sum_{n=1}^{N}\sum_{p=1}^{N-n} c_n^+ c_{n+p}^+\right]. \tag{2.27}$$

When developing the expression (2.27) we have taken into accaunt the fact, that the diagonal matrix elements of the odd number of Fermi operators are equal to zero.

Finally, going to the momentum representation:

$$c_n = \frac{\exp(-i\pi/4)}{\sqrt{N}}\sum_q e^{iqn}\eta_q\,,$$

and computing the matrix element for a fixed q after some an complicated transformations we arrive at the case of even states in the expression for the statistical sum $[Z_1^+(h)]$ (2.26):

$$\begin{aligned} Z_1^+(h) &= [2\cosh(h)]^N \prod_{0\le q\le\pi} \\ &\quad\times[\cosh 2K_2 - \sinh 2K_2\cos q + \alpha^2\sinh 2K_2(1+\cos q)] \\ &= [2\cosh(h)\cosh K_2]^N \prod_{n=1}^{N} \\ &\quad\times\left[1 + z_2^2 + 2z_2 z - 2z_2(1-z)\cos(\frac{2\pi n}{N})\right]^{1/2}, \end{aligned} \tag{2.28}$$

where $z_2 \equiv \tanh K_2$ and $z \equiv \alpha^2 = \tanh^2 h$. In the case of odd states it is easy to show that the sum $Z_1^-(h)$, is equal to $Z_1^-(h) = 2Z_1^+(h)$. Finally, we obtain in the thermodynamic limit again the formula (2.20), $(M \to N,\ \ K_1 \to K_2)$ for free energy per spin.

The $1D$ Ising model was discassed here with so many details because it was unexpectedly found, that $Z_1^+(h)$ such as represented in (2.28) can be applied in graph theory. Namely, using the representation (2.28) one can calculate the generating function for the Hamilton cycles on the simple square lattice $(N \times M)$, [9].

2.2. The 2D Ising model

For further purposes it is convenient to represent the matrix UT_2, entering the formula (2.18) and where U is defined by (2.14) in the form of a simple product of matrices P_n such that their diagonalization is relatively easy. The reason is that, as is known from [5] – [8], to calculate free energy per spin in the thermodynamic limit it is sufficient to find the maximal eigenvalue of the matrix UT_2, which is $2^N \times 2^N$ dimensional. First of all we note that the matrix U (2.14) can be represented in the form of a simple product of matrices U_0:

$$U = \prod_{n=1}^{N} U_n = U_0 \otimes U_0 \otimes ... \otimes U_0 \,, \quad N - \text{factors}\,, \tag{2.29}$$

where the matrix U_0 is defined by the formula (2.15), in which one should skip the index n. In order to represent the matrix T_2 (2.6) in the form of a simple product we will use the well known identity [10, 11]:

$$\exp(\mathbf{A}^2) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \exp(-\xi^2 + 2\mathbf{A}\xi) d\xi \,, \tag{2.30}$$

where $\mathbf{A}$ is a bounded operator (matrix). Writing $\exp(K_2 \sigma_n^z \sigma_{n+1}^z)$ in the form

$$\exp(K_2 \sigma_n^z \sigma_{n+1}^z) = \exp\left[\frac{K_2}{2}(\sigma_n^z + \sigma_{n+1}^z)^2 - K_2\right] \,.$$

we can represent the matrix T_2 in the form:

$$T_2 = \frac{e^{-NK_2}}{\pi^{N/2}} \int_{-\infty}^{\infty} .... \int_{-\infty}^{\infty}$$

$$\times \exp\left[-\sum_{n=1}^{N} \xi_n^2 + (2K_2)^{1/2} \sum_{n=1}^{N} (\xi_n + \xi_{n+1}) \sigma_{n+1}^z\right] \prod_{n=1}^{N} d\xi_n \,, \tag{2.31}$$

where $\sigma_{N+1}^z = \sigma_1^z$ and $\xi_{N+1} = \xi_1$. After writing the matrix T_2, (2.31) this way we can represent it in the form of a simple product of matrices $\exp[(2K_2)^{1/2}(\xi_n + \xi_{n+1})\sigma^z]$ inside the integral:

$$\prod_{n=1}^{N} \exp[(2K_2)^{1/2}(\xi_n + \xi_{n+1})\sigma_{n+1}^z] = \prod_{n=1}^{N} \otimes \exp[(2K_2)^{1/2}(\xi_n + \xi_{n+1})\sigma^z] \,, \tag{2.32}$$

where on the right hand side of the formula there is a simple product of 2×2 matrices. Next, we can write the matrix UT_2, using (2.29) and (2.31), (2.32), in the form:

$$UT_2 = \frac{e^{-NK_2}}{\pi^{N/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{n=1}^{N} d\xi_n$$
$$\times \exp\left[-\sum_{n=1}^{N} \xi_n^2\right] \left[\prod_{n=1}^{N} \otimes \exp[(2K_2)^{1/2}(\xi_n + \xi_{n+1})\sigma^z]\right], \quad (2.33)$$

where we included the constant matrix U under the integral and we used the known theorem on simple product of matrices:

$$(\mathbf{A_1} \otimes \mathbf{A_2} \otimes ...)(\mathbf{B_1} \otimes \mathbf{B_2} \otimes ...) = (\mathbf{A_1 B_1}) \otimes (\mathbf{A_2 B_2}) \otimes ....$$

Expression (2.33) enables the calculation of all 2^N eigenvalues of the matrix UT_2. Eigenvalues of the matrix $U_0 \exp[\alpha(\xi_n + \xi_{n+1})\sigma^z]$ can be easily calculated and are equal to:

$$\lambda^{\pm}(n, n+1) = e^{\pm\omega(n,n+1)}, \quad (2.34)$$

where $\omega(n, n+1)$ is defined as a positive root of the equation:

$$\cosh[\omega(n, n+1)] = \cosh(K_1^*) \cosh[h + \alpha(\xi_n + \xi_{n+1})], \quad \alpha \equiv (2K_2)^{1/2}. \quad (2.35)$$

In the diagonal representation the matrix V under the integral (2.33) can be represented in the form:

$$V = \left[\prod_{n=1}^{N} \otimes\ S(n, n+1)\right] \prod_{n=1}^{N}$$
$$\otimes \begin{pmatrix} \lambda^{+}(n, n+1) & 0 \\ 0 & \lambda^{-}(n, n+1) \end{pmatrix} \left[\prod_{n=1}^{N} \otimes S'(n, n+1)\right], \quad (2.36)$$

where $S(n, n+1)S'(n, n+1) = \mathbf{1}$, and $\lambda^{\pm}(n, n+1)$ are defined above by (2.34). From this it follows that the eigenvalues Λ_j of the matrix V are equal to:

$$\Lambda_j = \lambda^{\pm}(1, 2)\lambda^{\pm}(3, 4)...\lambda^{\pm}(N, 1), \quad (j = 1, 2, 3, ..., 2^N), \quad (2.37)$$

where to each j there corresponds a combination of $(+)$ and $(-)$ eigenvalues $\lambda^{\pm}(n\ , n+1)$.

Finally we can express the statistical sum (2.18) by the formula:

$$Z(h) = \mathrm{Tr}\left[(2\sinh 2K_1)^{N/2}\frac{e^{-NK_2}}{\pi^{N/2}}\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty}\prod_{n=1}^{N} d\xi_n \exp\left(-\sum_{n=1}^{N}\xi_n^2\right) V\right]^M, \tag{2.38}$$

where the matrix V is given by (2.36).

3. The free energy

As we mentioned above, the free energy per spin in the thermodynamic limit can be expressed by the maximal eigenvalue of the matrix UT_2, entering (2.18). We menaged to express this matrix in the form of an N-type integral (2.38), where the matrix V is defined by (2.36), and all the matrix elements of V are positive. On the other hand, in accordance with the known Frobenius–Perron theorem, the matrix B, with all, matrix elements positive has its maximal eigenvalue nondegenerate. Let us assign to the maximal eigenvalue of the matrix V a letter $\Lambda_{\max}$. In accordance with our definition of the eigenvalues $\lambda^{\pm}(n, n+1)$, using (2.37) we obtain the following expression for $\Lambda_{\max}$:

$$\Lambda_{\max} = \prod_{n=1}^{N}\lambda^{+}(n, n+1) = \prod_{n=1}^{N} e^{\omega(n, n+1)} = \exp\left[\sum_{n=1}^{N}\omega(n, n+1)\right], \tag{3.1}$$

where $\omega(n, n+1)$ is defined as a positive root of the equation (2.35), and

$$\Lambda_{\max} > \Lambda_j, \quad (j = 1, 2, \dots, 2^N).$$

Further we denote the eigenvalues of the matrix UT_2 by $\tilde{\Lambda}_j$. Taking into account the dimension of the matrix UT_2, which is equal to 2^N, we can write on the base of the relation (2.18) obvious inequalities:

$$\tilde{\Lambda}_{\max}^{M} \le Z(h) \le 2^N \tilde{\Lambda}_{\max}^{M}, \tag{3.2}$$

where $\tilde{\Lambda}_{\max}$ is the maximal eigenvalue in the set $\tilde{\Lambda}_j$, to which we also included also the constant factor $(2\sinh 2K_1)^{N/2}$. Taking the logarithm (3.2) of this expression and dividing by the nodes number NM, we arrive at the next system of inequalities:

$$\frac{1}{N}\ln(\tilde{\Lambda}_{\max}) \le \frac{1}{NM}\ln Z(h) \le \frac{1}{N}\ln(\tilde{\Lambda}_{\max}) + \frac{1}{M}\ln 2, \tag{3.3}$$

in which the expression in the middle represents free energy per node with accuracy to the factor $-\beta^{-1}$, where $\beta = \frac{1}{k_\beta T}$, T is temperature. Going to the limit $(N, M) \to \infty$, we obtain the desired formula describing free energy per spin in the thermodynamic limit:

$$f_2(h) = -\frac{1}{\beta} \lim_{N,M\to\infty} \frac{1}{NM} \ln Z(h) = -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N} \ln(\tilde{\Lambda}_{\max}) , \tag{3.4}$$

where $\tilde{\Lambda}_{\max}$ is, in accordance with (2.38) and (3.1) equal to:

$$\tilde{\Lambda}_{\max} = (2\sinh 2K_1)^{N/2} \frac{e^{-NK_2}}{\pi^{N/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{n=1}^{N} d\xi_n \times \exp\left[\sum_{n=1}^{N} (-\xi_n^2 + \omega(n, n+1))\right] . \tag{3.5}$$

Finally, using the Onsager identity:

$$| x | = \frac{1}{\pi} \int_0^{\pi} dq \ln[2\cosh(x) - 2\cos(q)] , \tag{3.6}$$

we obtain the following expression for the function $\omega(n, n+1)$ (2.35)

$$\omega(n, n+1) = \frac{1}{\pi} \int_0^{\pi} dq \ln[2\cosh K_1^* \cosh(h + (2K_2)^{1/2}(\xi_n + \xi_{n+1})) - 2\cos(q)] , \tag{3.7}$$

Expressions (3.4) and (3.5) should describe properly at least the transition to the one dimensional Ising model. It is easy to show that the transition to the limit $K_2 = 0$, gives the correct result (2.20) for the one dimensional Ising model. The analogous limit taken with respect to the constant K_1 seems a more complicated and has the form:

$$\lim_{K_1\to 0} \tilde{\Lambda}_{\max}(K_1) = \frac{e^{-NK_2}}{\pi^{N/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{n=1}^{N} d\xi_n \times \exp\left[-\sum_{n=1}^{N} \xi_n^2\right] \prod_{n=1}^{N} 2\cosh[h + \alpha(\xi_n + \xi_{n+1})] , \tag{3.8}$$

where α is defined above by (2.35). This is an integral of the Gauss type and it could be relatively easily calculated. For this purpose we apply the following formal procedure. Namely, let us write the expression $2\cosh(...)$, entering the integral (3.8), in the form:

$$2\cosh[h + \alpha(\xi_n + \xi_{n+1})] = \sum_{\mu_n=\pm 1} \exp[\mu_n h + \alpha\mu_n(\xi_n + \xi_{n+1})] , \quad (n = 1, 2, ..., N) , \tag{3.9}$$

where we introduced a new variable μ_n of the Ising type. Therefore, we can represent the right hand side of the equality (3.8) in the form:

$$\sum_{(\mu_n=\pm 1)} \left\{ \frac{e^{-NK_2}}{\pi^{N/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{n=1}^{N} d\xi_n \right.$$
$$\left. \times \exp\left[-\sum_{n=1}^{N} \xi_n^2 \right] \prod_{n=1}^{N} e^{h\mu_n} \exp[\alpha\mu_n(\xi_n + \xi_{n+1})] \right\}$$
$$= \sum_{(\mu_n=\pm 1)} \exp\left[\sum_{n=1}^{N} (h\mu_n + K_2\mu_n\mu_{n+1}) \right] , \quad (3.10)$$

where we took an integral over the variables ξ_n, and we imposed on variables μ_n cyclic boundary conditions ($\mu_{N+1} = \mu_1$). Calculation by standard methods [6, 7] of the sum (3.10), and following substitution of the expression (3.4), gives well known result (2.20).

Consideration of the expressions (3.4) and (3.5) for free energy of the twodimensional Ising model in external field we present at the end of this paper but now we go to the three dimensional case.

4. The three-dimensional Ising model

The Hamiltonian for the three dimensional Ising model in external field with nearest neighbors interaction we write in the form:

$$\mathcal{H} = - \sum_{(n,m,k)=1}^{NMK} \times \left(J_1\sigma_{nmk}\sigma_{n,m+1,k} + J_2\sigma_{nmk}\sigma_{n+1,mk} + J_3\sigma_{nmk}\sigma_{nm,k+1} + H\sigma_{nmk} \right) , \quad (4.1)$$

where the collective index (nmk) numbers nodes of the simple cubic lattice and H is the external field. Constants J_j take into account anisotropy of interaction of Ising spins. We impose on the variables σ_{nmk}, as it is commonly done, periodic boundary conditions. Quantities N, M and K are node numbers in corresponding directions of a cubic lattice. As is known [5], the statistical sum for the three dimensional Ising model can be represented in the form of a trace of the K-th power of the fiber–fiber transfer matrix (R):

$$W(h) = \mathrm{Tr}\,(R)^K \equiv \mathrm{Tr}\,(T_3T_2T_1T_h)^K , \quad (4.2)$$

where the matrices T_i, $(i = 1,2,3,h)$ of dimensions $2^{NM} \times 2^{NM}$ are of the form:

$$T_1 = \exp\left(K_1 \sum_{nm} \sigma^z_{nm}\sigma^z_{n,m+1}\right), \quad T_2 = \exp\left(K_2 \sum_{nm} \sigma^z_{nm}\sigma^z_{n+1,m}\right), \tag{4.3}$$

$$T_3 = (2\sinh 2K_3)^{NM/2} \exp\left(K_3^* \sum_{nm} \sigma^x_{nm}\right), \quad T_h = \exp\left(h \sum_{nm} \sigma^z_{nm}\right). \tag{4.4}$$

Here $K_i = \beta J_i$, $(i = 1,2,3)$; $\beta = (1/k_B T)$, T - temperature, $h = \beta H$, and K_3 and K_3^* are connected by relations of type (2.8). In the formulae (4.3)–(4.4) the matrices $\sigma^{x;z}_{nm}$ are Pauli matrices, which are defined analogously to (2.9), and have dimensions $2^{NM} \times 2^{NM}$.

Continuing considerations analogous to these in the two dimensional case we obtain the following formula describing free energy per spin in the thermodynamic limit:

$$f_3(h) = -\frac{1}{\beta} \lim_{N,M\to\infty} \frac{1}{NM} \ln \Lambda_{\max}, \tag{4.5}$$

where the maximal eigenvalue $\Lambda_{\max}$ of the matrix R, (4.2) is defined by:

$$\begin{aligned} \Lambda_{\max} &= (2\sinh 2K_3)^{NM/2} \frac{e^{-NM(K_1+K_2)}}{\pi^{NM}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{nm} d\eta_{nm} d\xi_{nm} \\ &\times \exp\left[\sum_{n,m=1}^{NM} \left(-\eta^2_{nm} - \xi^2_{nm} + \omega(n,m)\right)\right], \end{aligned} \tag{4.6}$$

and $\omega(n,m)$ is defined as the positive root of the equation:

$$\begin{aligned} \cosh\omega(n,m) &= \cosh K_3^* \cosh[h + \alpha_1(\eta_{n+1,m} + \eta_{n+1,m+1}) \\ &\quad + \alpha_2(\xi_{n,m+1} + \xi_{n+1,m+1})], \end{aligned} \tag{4.7}$$

where $\alpha_{1,2} = (2K_{1,2})^{1/2}$.

We impose on integration variables η_{nm} and ξ_{nm} cyclic boundary conditions, in accordance with periodic boundary conditions for the former variables:

$$\sigma^z_{N+1,m} = +\sigma^z_{1,m}, \quad \sigma^z_{n,M+1} = +\sigma^z_{n,1}, \quad n(m) = 1,2,3,\ldots N(M). \tag{4.8}$$

Similarly as in the twodimensional case, the function $\omega(n,m)$ can be expressed explicitly in terms of variables η_{nm} and ξ_{nm}, using for this aim the integral representation given by the Onsager identity (3.6).

It is slightly more complicated matter to take a limit with respect to the constant of interaction K_3, although the derived formula is much simpler than the formulae (3.4)–(3.5). Imposition of the limit ($K_3 \to 0$) in the formulae (4.5)–(4.7), gives, after some simple transformations, the following representation of free energy per spin of the two dimensional Ising model $f_2(h)$:

$$
\begin{aligned}
f_2(h) &= -\frac{1}{\beta}\left(\lim_{K_3\to 0,(N,M)\to\infty}\right)\frac{1}{NM}\ln \Lambda_{\max} \\
&= -\frac{1}{\beta}\lim_{(N,M)\to\infty}\frac{1}{NM} \\
&\times \ln\left\{\frac{e^{-NM(K_1+K_2)}}{\pi^{NM}}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{nm} d\eta_{nm}d\xi_{nm}\exp[-\sum_{nm}(\eta_{nm}^2+\xi_{nm}^2)]\right. \\
&\left.\times\prod_{nm} 2\cosh[h+\alpha_1(\eta_{n+1,m}+\eta_{n+1,m+1})+\alpha_2(\xi_{n,m+1}+\xi_{n+1,m+1})]\right\},
\end{aligned}
\tag{4.9}
$$

where we used relations of the type (2.8), and $\alpha_{1,2}$ are defined above (4.7). The integrals in (4.9) are integrals of the Gauss type and, as it is easy to show applying the described above formal way of introducing the variable of Ising type $\mu_{nm} = \pm 1$, can be represented in the form (2.2), what could lead to classical Onsager solution [2].

Analogously, one can show rigorously that free energy per spin for the threedimensional Ising model can be represented in the form of a multiple integral of the Gauss type:

$$
\begin{aligned}
f_3(h) = & -\frac{1}{\beta}\lim_{(N,M,K)\to\infty}\frac{1}{NMK} \\
&\times \ln\left\{\frac{e^{-NMK(K_1+K_2+K_3)}}{\pi^{3NMK/2}}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{nmk} d\eta_{nmk}d\xi_{nmk}d\zeta_{nmk}\right. \\
&\times \exp[-\sum_{n,m,k}(\eta_{nmk}^2+\xi_{nmk}^2+\zeta_{nmk}^2)] \\
&\times \prod_{nmk} 2\cosh[h+\alpha_1(\eta_{nmk}+\eta_{n+1,mk})+\alpha_2(\xi_{nmk}+\xi_{n,m+1,k}) \\
&\left.+\alpha_3(\zeta_{nmk}+\zeta_{nm,k+1})]\right\},
\end{aligned}
\tag{4.10}
$$

where $\alpha_i = (2K_i)^{1/2}$, $(i = 1, 2, 3)$. The formulae (4.10) can be an obviously generalized to describe d-dimensional Ising models but we will not consider the case here.

Let us make few remarks here. First of all, as far as it is known to the author, the representations for free energy per spin in the forms (3.4)–(3.5) and (4.5)–(4.10) for the two dimensional and threedimensional Ising models, respectively, have not appeared in the literature. We belive that the known representations (see, *e.g.* [12, 13]) are more complicated than the ones derived by us. The formulae (4.9) and (4.10) are, in a sense, obvious, the formulae (3.4)–(3.5) and (4.5)–(4.7) are not so. The integrals (3.5) and (4.6) can be represented as integrals of the "quasi Gauss" type, because the functions $\omega(n, n+1)$ and $\omega(n, m)$, described by the relations (2.35) and (4.7), respectively, in accordance with the Onsager identity (3.6) are almost "linear" in their arguments (ξ_n) and (η_{nm}, ξ_{nm}). This justifies our hopes that we it may be possible to calculate rigorously the integrals (3.5) and (4.6) in case $h = 0$ using an Ising type variable ($\mu = \pm 1$), described above. On the other hand, it seems that for the case ($h \neq 0$) it is much simpler to deal with the expression (3.5), than with the expression (4.9), although it could sound paradoxical. For the three dimensional Ising model in the external field ($h \neq 0$) the situation is no longer so clear, while for the infinitely small field ($h \sim 0$), similarly as in the two dimensional case, it is easier to analyze the expression (4.6), than (4.10).

5. Conclusions

The derived expressions (3.4)–(3.5) and (4.5)–(4.10) for free energy per spin for the Ising model can be of some interest, we hope. Actually, as can be seen from (3.4) and (4.5), we should learn how to calculate logarithmic asymptotics of multiple integrals of Gauss type. It is known, that there exist a well developed formalism of calculation of logarithmic asymptotes for integrals of the Laplace type for the one dimensional as well as for the multi dimensional cases [14]. In the case under consideration the situation is more complicated, because for the integrals of the kinds (3.4) and (4.5) it is not possible to transform them to a form of a multiple integral of the Laplace type, at least in the framework of their classical definition. With the increase of the large parameter ($\lambda \to \infty$) there also changes also the number of variables. over which one integrates and this needs reformulation of the corresponding methods of asymptotic estimation of the considered integrals [14]. In future publications we intended to investigate in more details the expressions (3.4) and (4.5), obtained in this paper and to calculate critical indices for the Ising model.

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REFERENCES

[1] E. Ising, *Z. Phys.* **31**, 253 (1925).
[2] L. Onsager, *Phys. Rev.* **65**, 117 (1944).
[3] C.N. Yang, *Phys. Rev.* **85**, 808 (1952).
[4] M. Gaudin, *La Fonction D'Onde De Bethe*, MASSON, Paris 1983.
[5] R.J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Academic Press, Inc., 1982.
[6] Yu.A. Izyumov, Yu.N. Skryabin: *Statistical Mechanics of Magnetically Ordered Systems*, Nauka, Moscow 1987 (in Russian).
[7] C.J. Thompson, *Classical Equilibrium Statistical Mechanics*, CLARENDON PRESS-OXFORD 1988.
[8] T.D. Schultz, D.C. Mattis, E.H. Lieb, *Rev. Mod. Phys.* **36**, 856 (1964).
[9] M.S. Kochmański, *J. Tech. Phys.* **37**, No 1, 67 (1996).
[10] J. Glimm, and A. Jaffe, *Quantum Physics*, Springer–Verlag, New York 1981.
[11] M.S. Kochmański, *J. Math. Ukr.* **46**, No 7, 857 (1994) (in Russian).
[12] B. McCoy, T.T. Wu, *Two Dimensional Ising Models*, Harvard U. Press. CAMBRIDGE 1973.
[13] E. Barouch, *Physica* **1D**, 333 (1980).
[14] M.V. Fedoryuk, *The Asymptotic, Integrals and Serieses*, SMB, Nauka, Moscow 1987 (in Russian).