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Nonanalytic Features of the First Order Phase Transition in the Ising Model

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Abstract. The absence of the analytic continuation for the free energy near the point of the first order phase transition in the d-dimensional Ising model is proved. It is shown that thermodynamic functions in the metastable phase do not have certain values and can be derived only with an uncertainty δ. The asymptotic expansion near the point of the phase transition yields the values of thermodynamic functions with the same uncertainty.

0. Introduction

The problem of existence of the analytic continuation for thermodynamic functions beyond the point of the first order phase transition is closely connected to the nature of metastable states. In the present work it will be shown that in the d-dimensional ($d \geqq 2$) ferromagnetic Ising model with nearest-neighbour interactions and for low temperatures there is no analytic continuation near the zero point of the magnetic field. Namely, let $F(E, h)$ be the free energy for the model where $E = 2 \cdot I/T$, $h = 2 \cdot H/T$, I is the energy of interaction, H is the magnetic field and T is the temperature. Then the following equality is the main result of this paper:

$$\lim_{h \to -0} \frac{1}{k!} \frac{\partial^k F}{\partial h^k} = (k!)^{\frac{1}{d-1}} (2(d-1)(E + C\xi))^{-\frac{kd}{d-1}},$$

where $k > E^d$, $C = C(d)$ depends only on the dimension and $|\xi| \leqq 1$ for sufficiently large E (see Sect. 3). The result will elucidate many features of the behaviour of the lattice gas in the metastable state.

A modification of the cluster expansion for the partition function will be used to obtain the main result. Two sets of terms with the same meaning will be defined. One of them can describe a wide class of lattice models, whereas the second class refers only to the Ising model with nearest-neighbour interactions. The question can be raised whether this double definition is necessary since only one model is considered. The fact is that the generalized partition function may refer both to the partition function of the model and to mathematical expressions which are not connected to any real physical system. One may notice that the mathematical induction applied in the theorems makes use of the nonphysical partition functions in certain steps. Therefore it is necessary to use generalized terms during the proofs of all theorems.

1. Contour Representation of the Partition Function

Let A_N denote a set of N elements and $\alpha_1, \alpha_2, \ldots$ be some subsets of $A_N(\alpha_1 \subset A_N, \alpha_2 \subset A_N, \ldots)$, which we call "contours." Each contour α has a complex weight W_α, and its order m_α is the number of elements in α. Two contours are considered to be joint if they have a common element $(\alpha_1 \cap \alpha_2 \neq \emptyset)$.

The definition of the generalized partition function (GPF) is as follows:

$$Z_N = 1 + \sum \prod_\alpha W_\alpha \tag{1.1}$$

when the sum is taken over all sets of non-joint contours and each term of the sum is the product of the weights in the set. GPF is a linear function of each weight W_α:

$$Z_N = Z'_N + W_\alpha Z_{N-m_\alpha}, \tag{1.2}$$

where $Z'_N = Z_{N|W_\alpha=0}$ and Z_{N-m_α} contains only contours not joint with α. In fact, Z_{N-m_α} is a GPF, based on $N-m_\alpha$ elements and on the contours containing only the elements of $A_N - \alpha$. The recurrent equation

$$Z_N = Z_{N-1} + \sum_\alpha W_\alpha Z_{N-m_\alpha} \tag{1.3}$$

is evident. Here an arbitrary element of A_N is fixed and the summation goes over all the contours containing the fixed element. Together with the condition $Z_0 = 1$, Eq. (1.3) may be considered as a definition of the GPF (1.1).

Concerning the Ising model, we first define the class of admissible volumes of the system, i.e. all the possible forms that lattice volumes can assume. By a square we mean a d-dimensional unit cube, by an edge we mean its $(d-1)$-dimensional face, and by a vertex we mean its $(d-2)$-dimensional face. Thus each square has $2d$ edges and $2d(d-1)$ vertices; an edge has $2(d-1)$ vertices and is joined to 2 squares; a vertex is joined to 4 squares and 4 edges. Two edges are connected, if they have a common vertex.

Let the volume Λ be a finite set of squares and Γ be the boundary of Λ; it means that all the edges of Γ separate Λ from the other squares in the lattice. Λ is defined as admissible, if Γ is a connected set of edges. Only admissible volumes and boundaries will be used later on. One can easily see that a volume can be determined when its boundary is given.

Now we make a correspondence between the model and the generalized terms. Namely, we identify the elements of a set with the vertices and the contours with the boundaries of the admissible volumes. The boundary Γ_α (contour α) is characterized by the following parameters: m_α is the number of vertices in Γ_α (the number of elements in the contour α), l_α is the number of edges in Γ_α (the length of Γ_α), s_α is the number of squares in Λ_α, having the boundary Γ_α (the area of Λ_α) and n_α is the number of vertices in Λ_α (except the m_α vertices in Γ_α). For instance, contour α (Fig. 1) has $m_\alpha = 21$, $l_\alpha = 22$, $s_\alpha = 16$, $n_\alpha = 6$.

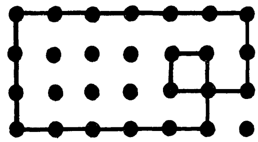

Fig. 1

In the Ising model every square (spin variable) can be in two states ± 1. A square is considered to be joint to the boundary if it contains one or more boundary vertices. We shall distinguish two types of boundary conditions: "+" and "−". In the first case all the internal squares, joint to Γ, have the fixed value $+1$ and vice versa. Volume Λ_α (Fig. 1) contains 14 boundary squares with fixed values and 2 free squares, taking part in the statistics. The corresponding model partition functions will be denoted as Z_Λ^+ and Z_Λ^-.

Now we are going to recall the definition of partition functions corresponding to different boundary conditions. The statistical weight of the state j (a configuration of ± 1 for the free squares) with "+" boundary condition is defined as $\exp(-EL_j + hS_j^-)$. Here S_j^- is the number of -1, L_j is the number of pairs of neighbouring squares with opposite values, E is real positive and h is a complex number. The statistical weight for "−" boundary condition is defined as $\exp(-EL_j - hS_j^+)$, where S_j^+ is the number of "+" squares in j. Z_Λ^+, Z_Λ^- are defined as the sums over all possible states j. The sums Z_Λ^+, Z_Λ^- differ from the generally accepted partition functions by unimportant factors which do not alter the results [3]. These definitions are used to get the following properties: 1) the weight of the non-perturbed state (the values of all squares are equal to that of the boundary squares) is 1, 2) $Z_\Lambda^+(h) = Z_\Lambda^-(-h)$. For example, $Z_\Lambda^+ = 1 + 2e^{-4E+h} + e^{-6E+2h}$, $Z_\Lambda^- = 1 + 2e^{-4E-h} + e^{-6E-2h}$ (Fig. 1).

Let M, L, S, N denote the parameters of the fixed boundary Γ_0 of the volume Λ_0. We identify the set of N internal vertices with the set A_N and all the internal boundaries $\Gamma_1, \Gamma_2, \ldots$ with the contours $\alpha_1, \alpha_2, \ldots$. Here we emphasize that only m_α (but not n_α) vertices are considered to belong to the contour α. Hence, the admissible boundaries in Λ_0 determine the subsets $\alpha_1, \alpha_2, \ldots$.

Now our aim is to define the weights of the contours (boundaries) in such a way that $Z_{\Lambda_0}^+ = Z_N$. The following two propositions are evident. Every state can be represented by a set of boundaries, separating "+" and "−" squares. Every set of boundaries without common vertices in all the pairs of boundaries represents a certain state. The weights W_{α_1}, $W_{\alpha_2}, \ldots$ for the case $h=0$ may be defined as $W_\alpha = \exp(-El_\alpha)$; then the equality $Z_{\Lambda_0}^+ = Z_N$ can be easily verified. In the more difficult case $h \neq 0$, we shall distinguish between weights $W_{\alpha_1}^+$, $W_{\alpha_2}^+, \ldots$ and $W_{\alpha_1}^-$, $W_{\alpha_2}^-, \ldots$, corresponding respectively to the "+" and "−" boundary conditions, and Z_N^+, Z_N^- as well. If the boundaries $\Gamma_1, \Gamma_2, \ldots$ are such that no boundary can include any other boundary (as it happened in the example), their weights are $W_\alpha^+ = \exp(-El_\alpha + hs_\alpha)$, $W_\alpha^- = \exp(-El_\alpha - hs_\alpha)$. However, when a boundary includes another one, the number of internal minuses or pluses depends on the presence of internal boundaries.

In order to obtain an equation for $Z_{\Lambda_0}^+$ we fix one internal vertex in the neighbourhood of the boundary Γ_0 and enumerate the possible cases:

$$Z_{\Lambda_0}^+(N) = Z_{\Lambda_0}^+(N-1) + \sum_\alpha e^{-El_\alpha - hs_\alpha} Z_{\Lambda_0 - \Lambda_\alpha}^+(N - m_\alpha - n_\alpha) Z_{\Lambda_\alpha}^-(n_\alpha). \qquad (1.4)$$

Here $Z^+_{\Lambda_0}(N-1)$ differs from $Z^+_{\Lambda_0}(N)$ in the following way: it does not contain any boundary Γ_α which includes the fixed vertex. The summation is taken over all such boundaries, $Z^+_{\Lambda_0-\Lambda_\alpha}(N-m_\alpha-n_\alpha)$ is the partition function of the volume $\Lambda_0-\Lambda_\alpha$, $Z^-_{\Lambda_\alpha}(n_\alpha)$ is the partition function of the volume with the boundary Γ_α. The partition function of two volumes is equal to the product of the partition functions. Therefore

$$Z^+_{\Lambda_0-\Lambda_\alpha}(N-m_\alpha-n_\alpha)Z^+_{\Lambda_\alpha}(n_\alpha)=Z^+_{\Lambda_0}(N-m_\alpha). \tag{1.5}$$

The definition

$$W_\alpha^+=\exp(-El_\alpha-hs_\alpha)Z^-_{\Lambda_\alpha}/Z^+_{\Lambda_\alpha} \tag{1.6}$$

allows us to rewrite (1.4) in the form of (1.3). Besides, $Z^+_{\Lambda_0}(0)=1$, so $Z^+_{\Lambda_0}(N)=Z^+_N$. Thus we have

$$\begin{aligned} W_\alpha^+&=\exp(-El_\alpha-hs_\alpha)Z^-_{n_\alpha}/Z^+_{n_\alpha},\\ W_\alpha^-&=\exp(-El_\alpha+hs_\alpha)Z^+_{n_\alpha}/Z^-_{n_\alpha}, \end{aligned} \tag{1.7}$$

with the following properties: $Z^+_N(h)=Z^-_N(-h)$, $W_\alpha^+(h)=W_\alpha^-(-h)$.

In the case of low temperatures (E is large) the phase transition exists in the point $h=0$, where the magnetization changes by a jump [2–5]. We shall suppose that $E>E_0$, E_0 is fixed and sufficiently large. According to the Lee-Yang theory [1–3] all zeroes of $Z^\pm_N$ correspond to the complex values of h, but in the thermodynamic limit some zeroes approach the point $h=0$. Our next aim is to obtain for any finite domain a circle $|h|\leqq r_0$, where the partition function has no zeroes.

The letter C with a subscript will be used as an estimate for the upper bound of a variable. It will be always assumed that 1) $C>0$, 2) $C=C(d)$ does not depend on volume, E, h, etc.; 3) if $C_1, C_2, \dots C_k$ have been already defined, we may increase C_k (if necessary) in all expressions; 4) E_0 may be defined only after all estimates C_1, $C_2, \dots$ have been introduced and it is sufficiently large in comparison with them. For instance, the number of contours with a fixed vertex and the fixed length $l_\alpha=l$ is less than C_1^l [2]. That will be the definition of C_1.

The letters θ (θ is complex, $|\theta|\leqq 1$) and ξ ($-1\leqq\xi\leqq 1$) will be used for writing inequalities in a more convenient form. For instance, $a-1\leqq b\leqq a+1$ and $a=b+\xi$ have the same meaning.

Further in all theorems Z^+_N, Z^-_N will stand for GPF with weights W_α^+, W_α^- (1.7). GPF may be equal to the Ising partition function for a certain volume or to a restricted partition function, where some contours are excluded (their weights are equal to the zero).

Theorem 1. *Let s_0 be the upper bound of the area of all contours in $Z^+_N: s_\alpha\leqq s_0$. Then,* $Z^+_N\neq 0$,

$$|\ln(Z^+_N/Z^+_{N-1})|<E^{-2}, \left|\frac{d}{dh}\ln(Z^+_N/Z^+_{N-1})\right|<E^{-2}, \tag{1.8}$$

$$|\ln(Z^+_N/Z^+_{N-m})|<mE^{-2}, \left|\frac{d}{dh}\ln(Z^+_N/Z^+_{N-m})\right|<mE^{-2}, \tag{1.9}$$

$$|\ln(Z^-_N/Z^+_N)|<2N|h|E^{-2}, \left|\frac{d}{dh}\ln(Z^-_N/Z^+_N)\right|<2NE^{-2} \tag{1.10}$$

in the circle $|h| \leqq r_0$, *where*

$$r_0 = 2dEs_0^{-1/d}/(1+C_2^{-1}). \tag{1.11}$$

The theorem is true for the negative boundary conditions as well.

Proof. The symmetry between "+" and "−" boundary conditions is evident. The inequality $Z_N^+ \neq 0$ follows from (1.8): it can be easily proved by mathematical induction on N. The inequalities (1.9) also can be obtained by using (1.8) m times. Inequalities (1.10) are obtained by using (1.8) $2N$ times; besides, 1) $Z_{N|N=0}^{\pm} = 1$, 2) $|f(z) - f(0)| \leqq |z| \cdot \max_\theta |f'(z\theta)|$ for an arbitrary analytic function $f(z)$, 3) $Z_N^- = Z_{N|h=0}^+$ must be taken into account.

The proof of (1.8) will be obtained with the help of mathematical induction on N, supposing that (1.8)–(1.10) are true for all N', $N' < N$, particularly for $Z_{n_\alpha}^{\pm}$ which are contained in the weights W_α^+ for Z_N^+. After dividing (1.3) by Z_{N-1}^+ we have:

$$Z_N^+/Z_{N-1}^+ = 1 + \sum_\alpha W_\alpha^+ Z_{N-m_\alpha}^+/Z_{N-1}^+. \tag{1.12}$$

Now we are able to obtain the upper bounds for the terms (1.12) and their derivatives with the help of (1.7), (1.9), (1.10):

$$\left|\frac{d}{dh}\ln W_\alpha^+\right| = \left|\frac{d}{dh}(-El_\alpha + hs_\alpha + \ln(Z_{n_\alpha}^-/Z_{n_\alpha}^+))\right| < s_\alpha + 2n_\alpha E^{-2},$$

$$\left|\frac{d}{dh}W_\alpha^+\right| < (s_\alpha + 2n_\alpha E^{-2})\,|W_\alpha^+|, \tag{1.13}$$

$$\left|\frac{d}{dh}(Z_{N-m_\alpha}^+/Z_{N-1}^+)\right| < (m_\alpha - 1)E^{-2}|Z_{N-m_\alpha}^+/Z_{N-1}^+|, \tag{1.14}$$

and

$$\left|\frac{d}{dh}(Z_N^+/Z_{N-1}^+)\right| = \left|\sum_\alpha \frac{d}{dh}(W_\alpha^+ Z_{N-m_\alpha}^+/Z_{N-1}^+)\right| < R_N.$$

Here

$$R_N = \sum_\alpha (s_\alpha + (2n_\alpha + m_\alpha - 1)E^{-2})\,|W_\alpha^+ Z_{N-m_\alpha}^+/Z_{N-1}^+|. \tag{1.15}$$

We can rewrite (1.9), (1.10) as

$$|Z_{N-m_\alpha}^+/Z_{N-1}^+| < \exp((m_\alpha - 1)E^{-2}) \tag{1.16}$$

and

$$|W_\alpha^+| < \exp(-El_\alpha + s_\alpha r_0 + 2n_\alpha r_0 E^{-2}). \tag{1.17}$$

Note that $n_\alpha < 2d(d-1)s_\alpha$, $m_\alpha < 2(d-1)l_\alpha$, $l_\alpha \geqq 2ds_\alpha^{(d-1)/d} \geqq 2ds_\alpha s_0^{-1/d}$, so that the following bound may be obtained from (1.16), (1.17):

$$\begin{aligned} |W_\alpha^+ Z_{N-m_\alpha}^+/Z_{N-1}^+| &< \exp(-El_\alpha + s_\alpha r_0(1+E^{-1}) + l_\alpha) \\ &\leqq \exp(-l_\alpha(E - 2C_2 - 1)/(C_2 + 1)), \end{aligned} \tag{1.18}$$

and thus

$$R_N < \sum_\alpha 2s_\alpha |W_\alpha^+ Z_{N-m_\alpha}^+ / Z_{N-1}^+|$$

$$< \sum_{l=2d}^{\infty} 2(l/2d)^{d/(d-1)} C_1^l \exp(-l(E-2C_2-1)/(C_2+1)) < \tfrac{1}{2}E^{-2} \quad (1.19)$$

(E_0 is sufficiently large). The comparison of (1.12) and (1.15) gives

$$1+R_N > |Z_N^+/Z_{N-1}^+| > 1-R_N > 1-\tfrac{1}{2}E^{-2},$$

and the first inequality (1.8). The second inequality (1.8) (and the last in the proof) follows from

$$\left|\frac{d}{dh}\frac{Z_N^+}{Z_{N-1}^+}\right| < \frac{1}{2}E^{-2} < \left|\frac{Z_N^+}{Z_{N-1}^+}\right| \cdot \frac{\tfrac{1}{2}E^{-2}}{1-\tfrac{1}{2}E^{-2}}.$$

2. Derivatives of Free Energy

Let Z_p^+ stand for the GPF of the square volume Λ_p: $S_p = p^d$, $L_p = 2d \cdot p^{d-1}$ with parameters M_p, L_p, S_p, N_p. Further on we shall write $[f]^{(k)}$ for the k^{th} derivative of any analytic function $f(h)$ at the point $h=0$:

$$[f]^{(k)} \equiv \left.\frac{d^k f}{dh^k}\right|_{h=0} \equiv \frac{k!}{2\pi i}\oint f(h)h^{-k-1}dh. \quad (2.1)$$

Theorem 2.

$$S_p^{-1}[\ln Z_p^+]^{(k)} = (k!(2(d-1)(E+C\xi))^{-k})^{d/(d-1)} \quad (2.2)$$

for arbitrary p, k with the restrictions $k > E^d$, and $p > (k/E)^{1/(d-1)}$.

Proof. We define the critical area S_0 as

$$S_0 = (k/2dE(1-C_2^{-1}))^{d/(d-1)}, \quad (2.3)$$

and enumerate all contours in Λ_p with the area $S_\alpha > S_0$: $\alpha_1, \alpha_2, \alpha_3, \ldots$. The order of the enumeration is arbitrary but it is required that $S_{\alpha_1} \leqq S_{\alpha_2} \leqq S_{\alpha_3} \leqq \ldots$. Let Z_i^+ stand for a restricted GPF: Z_i^+ contains only "small" contours with $S_\alpha \leqq S_0$ and contours $\alpha_1, \alpha_2, \ldots \alpha_i$; Z_0^+ contains only "small" contours. It is evident that

$$\ln Z_p^+ = \ln Z_0^+ + \sum_i U_i, \quad (2.4)$$

where U_i is defined as $U_i = \ln(Z_{i+1}^+/Z_i^+)$ $(i=0,1,2,\ldots)$.

Our aim is to prove that $[U_i]^{(k)} > 0$ and $|[\ln Z_0^+]^{(k)}|$ is sufficiently small. In order to examine $[U_i]^{(k)}$ we fix an arbitrary contour α_{i+1}. Its parameters will be written simply as M, L, S, N. In this case Eq. (1.2) has the form

$$Z_{i+1}^+ = Z_i^+ + W_{\alpha_{i+1}}^+ Z_i^{+R}. \quad (2.5)$$

Here Z_i^{+R} is a restriction of Z_i^+ (Z_i^{+R} does not contain the M vertices belonging to α_{i+1} nor the contours joined to α_{i+1}). Whence,

$$U_i = \ln(1+V_i) = V_i - \tfrac{1}{2}V_i^2 + \tfrac{1}{3}V_i^3 - \ldots, \quad (2.6)$$

where $V_i = W_{\alpha_{i+1}}^+ Z_i^{+R}/Z_i^+$. The bounds for $[V_i]^{(k)}$, $[V_i^2]^{(k)}, \ldots$, can be derived from the following theorem.

Theorem 3. *Let $f(z)$ stand for an analytic function in the circle $|z|<R$, where $|f'(z)|\leqq A$, $A<1/4$ and $f(z)$ is real for real z. In this case the coefficient a_k $(R\cdot(1-2\sqrt{A})>k>100)$ of the expansion $e^{z+f(z)}=a_0+a_1z+a_2z^2+\ldots$ satisfies the inequalities*

$$\tfrac{1}{12}e^{r+f(r)}r^{-k-1/2}<a_k<e^{r+f(r)}r^{-k-1/2}, \tag{2.7}$$

where r is the unique positive $(0<r<R)$ solution of the equation

$$r(1+f'(r))=k. \tag{2.8}$$

The proof is given in the Appendix.

In order to use Theorem 3 in our case we consider $z=nSh$,

$$f(z)=n(\ln(Z_N^-/Z_N^+)+\ln(Z_i^{+R}/Z_i^+)-EL), \tag{2.9}$$

where n is a fixed positive integer $(n=1,2,3,\ldots)$. Taking into account the definition of V_i and $W_{\alpha_{i+1}}^+$, we obtain $\exp(z+f(z))=V_i^n$. Since $f(z)$ is an analytic function inside the circle of radius $R=n\cdot S\cdot r_0$, where r_0 is given by

$$r_0=2\cdot d\cdot E\cdot S^{-1/d}/(1+C_2^{-1}) \tag{2.10}$$

[cf. with Eq. (1.11)], Theorem 3 can be applied. Now

$$\begin{aligned}|f'(z)|&=S^{-1}\left|\frac{d}{dh}\ln(Z_N^-/Z_N^+)+\frac{d}{dh}\ln(Z_i^{+R}/Z_i^+)\right|\\&<S^{-1}(2N+M)E^{-2}<E^{-1}.\end{aligned}$$

Therefore A can be defined as $A=E^{-1}$. Choosing, for example $E_0>10$, both $A>1/4$ and $k>100$ will be satisfied. (Remember that $k>E^d$.) Besides,

$$\begin{aligned}R(1-2\sqrt{A})&=nSr_0(1-2E^{-1/2})>2dES_0^{(d-1)/d}(1-2E^{-1/2})/(1+C_2^{-1})\\&=k(1-2E^{-1/2})/(1-C_2^{-2})>k.\end{aligned}$$

The requirements of Theorem 3 are fulfilled so that we can write the inequalities (2.7) for $a_k=n^{-k}S^{-k}[V_i^n]^{(k)}/k!$. From Eq. (2.8) one gets $k/(1+E^{-1})<r<k/(1-E^{-1})$ or $r=k/(1+\xi/E)$.

Now we rewrite (2.7) in a more convenient form, noting that a constant (such as $\sqrt{2\pi}$ or λ: $1/12<\lambda<1$) can be written as $\exp(\xi k/E)$, when $k>E^d$. We obtain $r^{-k}=k^{-k}\exp(3\xi k/2E)$ and $\lambda r^{-k-1/2}e^r=\exp(3\xi k/E)/k!$. Besides, from Theorem 1 we get

$$|\ln(Z_N^-/Z_N^+)|<\frac{2Nr_0}{E^2}=\frac{4dNS^{(d-1)/d}}{ES(1+C_2^{-1})}\leqq\frac{2NL}{ES(1+C_2^{-1})}<\frac{L}{2},$$

and

$$|\ln(Z_i^{+R}/Z_i^+)|<M/E^2<L/2,$$

and hence $\exp f(r)=\exp(n\cdot L\cdot(\xi-E))$. Taking into account that

$$L\geqq 2dS^{(d-1)/d}>2dS_0^{(d-1)/d}=k/E(1-C_2^{-1})>k/E, \tag{2.12}$$

we finally obtain

$$a_k=\exp(nL(4\xi-E))/k!,\,[V_i^n]^{(k)}=n^kS^k\exp(nL(4\xi-E)). \tag{2.13}$$

In order to obtain similar estimates for $[U_i]^{(k)}$, we use the inequality

$$[V_i^n]^{(k)}/[V_i]^{(k)} < n^k \exp((1-n)EL + 4(1+n)L) < 2^{-n}$$

(notice that $E \cdot L > k$). From the expansion (2.6) we obtain

$$\tfrac{1}{2}[V_i]^{(k)} < [U_i]^{(k)} < \tfrac{3}{2}[V_i]^{(k)}, \ [U_i]^{(k)} = S^k \exp(5L\xi - LE). \tag{2.14}$$

This formula enables us to get estimates for the k^{th} derivative of the sum (2.4). The function $\psi(S, L) = S^k e^{-L \cdot E}$ takes on its maximum for square contours defined by $S = q^d$, $L = 2dq^{d-1}$. Now $\psi(q) = q^{kd} \exp(-2dq^{d-1} \cdot E)$ is maximal for $q = q_m$, where

$$q_m = (k/2(d-1)E)^{1/(d-1)}. \tag{2.15}$$

Then

$$L_m = dk/(d-1)E, \psi_m = \psi(q_m) = (k/2eE(d-1))^{dk/(d-1)}. \tag{2.16}$$

Attention should be paid to the fact that q_m is not natural, whereas $q = 1, 2, 3, \ldots$. Hereafter we use $q'_m = [q_m]$, i.e. the integer part of q_m. The inequality $\psi'_m = \psi(q'_m) > \psi_m \exp(-2dk/E)$ can be obtained after a simple calculation. The square volume with $p > (k/E)^{1/(d-1)}$ contains not less than $S_p/5$ square contours with the side q'_m. Therefore, since L_m, ψ_m obey (2.15) and (2.16), we get

$$\sum_i [U_i]^{(k)} > \frac{S_p}{5} \left(\frac{k}{2eE(d-1)}\right)^{\frac{dk}{d-1}} \exp\left(-\left(\frac{5d}{d-1} + 2d\right)\frac{k}{E}\right). \tag{2.17}$$

The upper estimate for the sum (2.17) will be obtained when all the contours with the fixed length $l_\alpha = L$ will be collected. The weight of each class is defined as $U_L^\Sigma = \sum_i U_{i|l_i = L}$. The number of contours in every class is less than $S_p \cdot C_1^L$ and $S_\alpha \leqq (L/2d)^{d/(d-1)}$. Therefore,

$$[U_L^\Sigma]^{(k)} < S_p C_1^L (L/2d)^{dk/(d-1)} e^{5L - EL}. \tag{2.18}$$

Summation of (2.18) over L yields

$$\sum_i [U_i]^{(k)} < \sqrt{k} S_p \left(\frac{k}{2e(d-1)(E - 5 - \ln C_1)}\right)^{dk/(d-1)}, \tag{2.19}$$

where we used the inequality

$$\sum_{L=1}^{\infty} e^{-Lq} L^p < \frac{2\sqrt{2\pi p}}{q} \left(\frac{p}{eq}\right)^p \qquad (q > 1, p > 1).$$

The bounds (2.17), (2.19) can be united in the equation

$$\sum_i [U_i]^{(k)} = S_p (2e(d-1)(E + C_3 \xi)/k)^{-dk/(d-1)}. \tag{2.20}$$

Finally, it is necessary to show that $|[\ln Z_0^+]^{(k)}|$ is less than half of the bound (2.17); then, according to (2.4), the bounds (2.20) will remain true for $[\ln Z_p^+]^{(k)}$ with C_3 replaced by C_4. Taking into account that $\ln Z_0^+$ is an analytic function inside the circle $|h| < r_0$ (1.11) for S_0, given by (2.3), we have

$$|[\ln Z_0^+]^{(k)}| < k! S_p r_0^{-k} = k! S_p \left(\frac{k(1 + C_2^{-1})^{d-1}}{(2dE)^d (1 - C_2^{-1})}\right)^{k/(d-1)}, \tag{2.21}$$

where the estimate $|\ln Z_0^+| < S_p$ is used. The comparison between (2.20) and (2.21) together with $k! < 3\sqrt{k}(k/e)^k$ gives the necessary statement. Equation (2.2) is a more convenient form of (2.20).

3. Thermodynamic Limit

Theorem 2 shows the behaviour of the derivatives of the free energy $F_p = S_p^{-1} \ln Z_p^+$ for arbitrarily large but finite systems. However, we cannot say at once that the derivatives $F^{(k)} = \lim_{h \to -0} \frac{\partial^k F}{\partial h^k}$ of the free energy $F = \lim_{p \to \infty} F_p$ obey the same estimates, because we can say nothing about the change of order of limits $p \to \infty$ and $h \to -0$. In this section it will be shown that the limits exist and can be interchanged: $F^{(k)} = \lim_{p \to \infty} [F_p]^{(k)}$. In fact it is sufficient to find a region on the complex plane h having the boundary point $h = 0$, where $Z_p^+ \neq 0$ and $\frac{\partial^k F_p}{\partial h^k}$ is uniformly bounded for all p and h. The Lee-Yang circle theorem [1, 2] yields a region $|e^h| < 1$, where $Z \neq 0$ but without any requirement imposed on $\frac{\partial^k F_p}{\partial h^k}$.

Let Λ_0 be an arbitrary admissible volume with the parameters M, L, S, N, and let Z_N^+ be the corresponding partition function. We fix an arbitrary natural number q $(q = 1, 2, 3, \ldots)$, and among the contours in Λ_0 we distinguish the "small" contours, satisfying $s_\alpha \leqq q^d$. The subscript β will be used to label the "large" contours $(s_\beta > q^d)$, and α is used for the small ones. Let Z_N^{+*}, Z_N^{-*} be restricted partition functions containing only small contours. Thus Eqs. (1.3) will be

$$Z_N^+ = Z_{N-1}^+ + \sum_\alpha W_\alpha^+ Z_{N-m_\alpha}^+ + \sum_\beta W_\beta^+ Z_{N-m_\beta}^+ \tag{3.1}$$

and

$$Z_N^{+*} = Z_{N-1}^{+*} + \sum_\alpha W_\alpha^+ Z_{N-m_\alpha}^{+*}. \tag{3.2}$$

Similar equations can be written for Z_N^- and Z_N^{-*}, but a somewhat different formulation will be used. Let j stand for a set of large external contours, i.e. having the property that none of the contours in the set j contains (in its interior) or is joined to any other contour of the set j. The corresponding parameters m_j, l_j, s_j, and n_j are the sums of m_β, l_β, s_β, and n_β respectively. With this notation we have

$$Z_N^- = Z_N^{-*} + \sum_j \left(Z_{N-m_j-n_j}^{-*} \prod_\beta Z_{n_\beta}^+ e^{-l_\beta E - s_\beta h} \right), \tag{3.3}$$

where the product is taken over all the contours β belonging to j.

Lemma 1. *The number of sets j for the volume Λ_0 with fixed $l_j = l_0$ and $s_j = s_0$ is less than* $\exp(C_5(L + l_0 + l_q))$, *where* $l_q = d \cdot (S - s_0)/(q+1)$.

Proof. It is sufficient to show that for every j we need at most l_q additional edges in the volume $\Lambda_0 - \Lambda_j$ in order to connect all the internal large contours (belonging to j) with the external contour Γ_0 (the boundary of Λ_0). Performing this, we have a joined system of edges with a total length $L + l_0 + l_q$, whereas the number of joint systems of l edges is bounded by $\exp(l \cdot C_5)$.

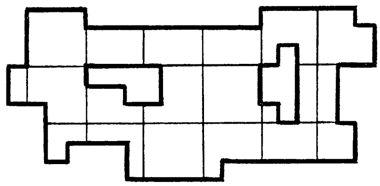

Fig. 2

Let $x_1, \ldots, x_d$ be the basic vectors of the lattice. The total length of the edges (surface of hyperplanes in the d-dimensional case) normal to x_1 in $\Lambda_0 - \Lambda_j$ is less than $S - s_0$. Let us collect these edges (hypersquares) in straight lines (hyperplanes) perpendicular to x_1 and draw the lines not with step 1 but with step $q+1$ (the others will be omitted). There are still $q+1$ possibilities because of the translations in the direction of x_1, but we take the one for which the minimum of additional edges is needed. This minimum is less than $(S - s_0)/(q+1)$. When this procedure is repeated for the rest of $d-1$ vectors $x_2, \ldots, x_d$, the number of additional edges will be less than l_q. Thus the volume $\Lambda_0 - \Lambda_j$ will be divided into square volumes. Every contour $\beta \in j$ will be linked to the boundary Γ_0 with the additional edges, because $s_\beta > q^d$ (see Fig. 2, where $q=2$).

Theorem 4. *The inequalities*

$$Z_N^+ \neq 0\,,$$
$$|\ln(Z_N^+/Z_{N-1}^+) - \ln(Z_N^{+*}/Z_{N-1}^{+*})| < HE^{-2} \tag{3.4}$$

and

$$|W_\alpha^+| < \exp((C_5 - E)l_\alpha)\,, \qquad |W_\beta^+| < \exp((C_5 - E)l_\beta) \tag{3.5}$$

hold true in the sector D^+*:* $\pi/2 + C_6/2E < \arg h < 3\pi/2 - C_6/2E$. *Here* $H = \min(|h|, 1)$, $q = [2dE/(1 + C_2^{-1})\,|h|]$.

Proof. The proof is based on mathematical induction on N. At first, we prove (3.5) and $Z_N^+ \neq 0$ by assuming that (3.4) holds with N replaced by n_α and n_β. The second step is to prove (3.4), when the weights for Z_N^+, Z_N^{+*} can be estimated by (3.5).

Let us notice that the parameter $q = q(h)$ is chosen so that the point h ($h \in D^+$) belongs to the circle $|h| < r_0$, given in Theorem 1, when $s_0 = q^d$. It means that for every fixed h ($h \in D^+$) we classify the contours as small and large and define Z_N^{+*} ($s_\alpha \leqq q^d$) so that the requirements of Theorem 1 are satisfied. Thus, $Z_N^{+*} \neq 0$, $Z_{N-1}^{+*} \neq 0$, and the inequality $Z_N^+ \neq 0$ is derived from (3.4) and from $Z_{N-1}^+ \neq 0$ by induction on N.

Dividing the Eq. (3.3) by Z_N^+ we have

$$\frac{Z_N^-}{Z_N^+} = \frac{Z_N^{-*}}{Z_N^+} + \sum_j \frac{Z_{N-m_j-n_j}^{-*} Z_{N-m_j}^+}{Z_{N-m_j-n_j}^+ Z_N^+} e^{-l_j E - s_j h}\,, \tag{3.6}$$

where we used

$$Z_{N-m_j}^+ = Z_{N-m_j-n_j}^+ \prod_\beta Z_{n_\beta}^+\,.$$

On the other hand inequality (3.4) can be written as

$$Z_{N-1}^+ Z_N^{+*} / Z_N^+ Z_{N-1}^{+*} = e^{H\theta/E^2}\,, \tag{3.7}$$

and iterating (3.7) m times and N times, respectively, one gets

$$\frac{Z_{N-m}^{+}Z_{N}^{+*}}{Z_{N}^{+}Z_{N-m}^{+*}}=e^{mH\theta/E^2} \quad\text{and}\quad \frac{Z_N^{+*}}{Z_N^{+}}=e^{NH\theta/E^2}. \tag{3.8}$$

According to Theorem 1,

$$Z_N^{+*}/Z_{N-m}^{+*}=e^{m\theta/E^2} \quad\text{and}\quad Z_N^{-*}/Z_N^{+*}=e^{2NH\theta/E^2},$$

therefore we find

$$Z_{N-m}^{+}/Z_N^{+}=e^{2m\theta/E^2} \quad\text{and}\quad Z_N^{-*}/Z_N^{+}=e^{3NH\theta/E^2}. \tag{3.9}$$

This enables us to obtain upper bound for (3.6):

$$|e^{Sh}Z_N^{-}/Z_N^{+}|<\exp(3NH/E^2+S\,\mathrm{Re}\,h) + \sum_j \exp(3(N-m_j-n_j)H/E^2+2m_j/E^2-l_jE+(S-s_j)\,\mathrm{Re}\,h). \tag{3.10}$$

Now, by using the estimates of Lemma 1 we have

$$\begin{aligned}|e^{Sh}Z_N^{-}/Z_N^{+}|&<\exp(S(6d(d-1)\,|h|/E^2+\mathrm{Re}\,h))\\ &\quad+e^{LC_5}\sum_{l=2d}^{\infty}\sum_{s'}\exp(s'(6d(d-1)\,|h|/E^2+\mathrm{Re}\,h+dC_5/(q+1))\\ &\quad+l(C_5+4(d-1)/E^2-E)),\end{aligned}$$

where $s'=S-s_j$ and $1\leqq S-s'\leqq(l/2d)^{d/(d-1)}$. Besides, we used $N<2d(d-1)S$, $N-m_j-n_j<2d(d-1)s'$ and $m_j<2(d-1)l_j$. The choice of q yields $d/(q+1)<|h|/E$. Region D^+ possesses the following property:

$-\mathrm{Re}\,h/|h|>C_6/3E$, where C_6 is not fixed yet.

Let us put $C_6=1+3C_5$. In this case, $6d(d-1)\,|h|/E^2+\mathrm{Re}\,h+dC_5/(q+1)<0$ and

$$|e^{Sh}Z_N^{-}/Z_N^{+}|<1+e^{LC_5}\sum_{l=2d}^{\infty}(l/2d)^{d/(d-1)}\exp(l(C_5+4(d-1)/E^2-E))<e^{LC_5}.$$

A comparison with the definition (1.7) of the weights results the inequality (3.5).

It remained to prove (3.4), assuming that (3.5) holds for the weights W_α^+, W_β^+, appearing in Z_N^+ and Z_N^{+*}. Equations (3.1) and (3.2) give

$$Z_N^{+}/Z_{N-1}^{+}-Z_N^{+*}/Z_{N-1}^{+*}=\sum_\alpha W_\alpha^+(Z_{N-m_\alpha}^{+}/Z_{N-1}^{+} - Z_{N-m_\alpha}^{+*}/Z_{N-1}^{+*})+\sum_\beta W_\beta^+Z_{N-m_\beta}^{+}/Z_{N-1}^{+}. \tag{3.11}$$

Then, from (3.5), (3.8), (3.9) and $2m_\beta/E^2<l_\beta$, it follows that

$$|W_\beta^+Z_{N-m_\beta}^{+}/Z_{N-1}^{+}|<e^{l_\beta(C_5+1-E)} \tag{3.12}$$

and

$$\left|W_\alpha^+\left(\frac{Z_{N-m_\alpha}^{+}}{Z_{N-1}^{+}}-\frac{Z_{N-m_\alpha}^{+*}}{Z_{N-1}^{+*}}\right)\right|=\left|W_\alpha^+\frac{Z_{N-m_\alpha}^{+*}}{Z_{N-1}^{+*}}\left(\frac{Z_{N-m_\alpha}^{+}Z_{N-1}^{+*}}{Z_{N-1}^{+}Z_{N-m_\alpha}^{+*}}-1\right)\right|$$

$$<e^{l_\alpha(C_5+1-E)}(e^{m_\alpha H/E^2}-1)<e^{l_\alpha(C_5+2-E)}(1-e^{-l_\alpha H})<H\,e^{l_\alpha(C_5+2-E)}.$$

The number of contours with $l_\alpha = l$ is bounded by C_1^l, therefore, the first sum in (3.11) is less than $H/4E^2$ and the second sum is less than $1/4E^2 l_{\beta\,\min}$, where $l_{\beta\,\min}$ is the minimum of the length of the large contours for a given q. It is easy to show that with the particular choice of $q\, l_{\beta\,\min}^{-1} < H$: if $H=1$ we have $l_{\beta\,\min}^{-1} < H$, because $l_\beta > 1$, and when $H=|h|<1$ we obtain, that $q > E/|h|$, $l_{\beta\,\min} > q$ and $l_{\beta\,\min}^{-1} < H$. In this way,

$$|Z_N^+/Z_{N-1}^+ - Z_N^{+*}/Z_{N-1}^{+*}| < H/2E^2\,. \tag{3.13}$$

The identity

$$\frac{Z_N^+ Z_{N-1}^{+*}}{Z_{N-1}^+ Z_N^{+*}} = 1 + \frac{Z_{N-1}^{+*}}{Z_N^{+*}}\left(\frac{Z_N^+}{Z_{N-1}^+} - \frac{Z_N^{+*}}{Z_{N-1}^{+*}}\right)$$

together with Theorem 1 gives

$$1 - e^{E^{-2}} H/2E^2 < \left|\frac{Z_N^+ Z_{N-1}^{+*}}{Z_{N-1}^+ Z_N^{+*}}\right| < 1 + e^{E^{-2}} H/2E^2 \tag{3.14}$$

and (3.4) follows from (3.14).

Corollary 1. *Let Λ_n be an increasing sequence of admissible volumes and assume that the corresponding free energies $F_{\Lambda_n}(h)$ converge for real negative h. Then F_{Λ_n} converges to an analytic function $F(h)$ in the region D^+.*

The Lee-Yang theorem gives the same result, but without the restrictions (3.4), (3.5).

Corollary 2. *The results of Theorem 4 remain valid for negative boundary conditions in the region D^-:*

$$-\pi/2 + C_6/2E < \arg h < \pi/2 - C_6/2E\,.$$

Let D_1^+ stand for the region $\pi/2 + C_6/E < \arg h < 3\pi/2 - C_6/E$. Thus, D_1^+ is contained in D^+ $(D_1^+ \subset D^+)$.

Theorem 5.

$$\lim_{p\to\infty} [F_p]^{(k)} = \lim_{h\to 0} \frac{\partial^k F}{\partial h^k} \tag{3.15}$$

is valid for arbitrary k $(k=1,2,3,\ldots)$ and $h\in D_1^+$.

Proof. At first, we prove that the derivative $\dfrac{\partial^k F_p}{\partial h^k}$ is uniformly bounded for all p and $h \in D_1^+$. We consider Λ_p with the parameters M_p, L_p, S_p, N_p and use the definitions of Sect. 2 for Z_0^+, Z_1^+, $Z_2^+, \ldots$, $U_i = \ln(Z_{i+1}^+/Z_i^+)$, $U_i = \ln(1+V_i)$ and $V_i = W_{\alpha_{i+1}}^+ Z_i^{+R}/Z_i^+$. The only difference is that now we put $S_0 = 0$, and thus all the contours are numbered. Whence, $Z_0^+ = 1$ and $Z_p^+ = \sum_i U_i$. For a fixed contour α_{i+1} with the parameters M, L, S, N we have

$$|V_i| < \exp(-L(E - 2C_2 - 1)/(C_2 + 1))$$

in the circle (2.10), according to (1.18). Theorem 4 gives the inequality (3.12) $|V_i| < \exp(-L(E - C_5 - 1))$ for $h \in D^+$. Therefore, $|U_i| < \exp(-LE/2C_2)$ if $h \in D_0^+$, where $D_0^+ = D^+ \cup D_0$ and $D_0 : |h| < r_0$. One can easily see that $D_1^+ \subset D_0^+$, and the distance between the boundaries of D_0^+ and D_1^+ is not less than $\delta = r_0 C_6/3E$. The Cauchy formula for the k^{th} derivative on the complex plane gives

$$\left|\frac{\partial^k U_i}{\partial h^k}\right| < U_{ik}, \qquad U_{ik} = k!\,\delta^{-k}\exp(-LE/2C_2)$$

for arbitrary $h \in D_1^+$. We define $U_k^\Sigma = \sum_i U_{ik}$, when the summation is taken over all the translationally non-equivalent contours on the infinite lattice. It is evident that the series $\sum_i U_{ik}$ converges. Each contour in the volume Λ_p has less than S_p translations in Λ_p, so we conclude that $\left|\frac{\partial^k F_p}{\partial h^k}\right| < U_k^\Sigma$ for $h \in D_1^+$. Notice that U_k^Σ does not depend on p and h (but it depends on k).

The following proposition will help us to finish the proof. Let the functions $f_1(x), f_2(x), f_3(x), \ldots$ have the second derivatives uniformly bounded for all n and $a \leqq x \leqq b$:

$|f_n''(x)| \leqq A$, and suppose that $f_n(x) \to f(x)$. In this case $f(x)$ has a continuous derivative and $\lim_{n\to\infty} f_n'(a) = \lim_{x\to a} f'(x)$.

All the derivatives of F_p are bounded and thus we obtain (3.15).

Corollary.

$$\lim_{h\to 0} \frac{1}{k!}\frac{\partial^k F}{\partial h^k} = A_k, \qquad A_k = (k!)^{1/(d-1)}(2(d-1)(E+C\xi))^{-kd/(d-1)}, \tag{3.16}$$

where $h \in D_1^+$, $k > E^d$, and therefore the series $F^+(h) \sim A_0 + A_1 h + A_2 h^2 + \ldots$ does not converge for any $h \neq 0$. Hence, $h = 0$ is a non-analytic point of $F(h)$.

4. Discussion

The Ising model can be interpreted as a model of a lattice gas with the chemical potential h and interaction E, where each negative square corresponds to a molecule. In this case $F(h, E)$ is the pressure and $\frac{\partial F}{\partial h}$ is the density. The gaseous phase corresponds to the negative values of h and the liquid phase corresponds to $h > 0$. The zero value of h is the point of the first order phase transition [2–5], when the density changes by a jump.

The results of Theorems 1, 2, and 5 enable us to make some conclusions about the nature of the metastable states. The metastable phase is usually interpreted by supposing the existence of the analytic continuation of the pressure through the phase transition point and all thermodynamic functions in the metastable phase are defined with the help of this analytic continuation. According to this interpretation, the behaviour of the thermodynamic functions does not make it possible to remark that the system approaches the point of a phase transition until we pass it. Only the partition function has some peculiar behaviour near this point.

The absence of the analytic continuation for the Ising model makes it necessary to investigate the problem of the definition of the thermodynamic functions in the metastable phase. We fix a sufficiently large square volume Λ_p with "+" boundary conditions, h being positive and $h \ll E$. Positive values of h correspond to a liquid phase, whereas the "+" boundary condition compels the system to remain in the gaseous state. "Sufficiently large volume" means that the main contribution to the partition function is given by the configurations corresponding to the liquid phase. All these configurations may be represented with the help of a large contour containing almost all the volume and a few small contours within this large one.

The partition function for the gaseous metastable phase may be defined as a restricted sum over configurations, when all configurations with large contours are excluded. Now it is necessary to define a difference between large and small contours. The weight of the configuration with only one contour α is $P_\alpha = \exp(-El_\alpha + hs_\alpha)$. We assume that the area s_α can increase in such a way that $s_\alpha = s_0 q^d$ and $l_\alpha = l_0 q^{d-1}$, where q is a parameter and s_0, l_0 are constants. The function $P_\alpha = P_\alpha(q)$ first decreases $(0 < q < q_m,\ q_m = (d-1) l_0 E / d s_0 h)$ and then increases $(q > q_m)$. If this contour is interpreted as a (liquid) drop, then we may say that the contour $\alpha|_{q=q_m}$ is a critical droplet which realizes a transition from the metastable gaseous phase to the stable liquid one. The critical weight $P_m = P_\alpha(q_m)$ depends on the ratio s_0/l_0 and reaches its maximum for square contours, where $s_\alpha = q^d$, $l_\alpha = 2dq^{d-1}$, $q_{mm} = 2(d-1)E/h$ and $P_{mm} = P_\alpha(q_{mm}) = \exp(-2^d E^d ((d-1)/h)^{d-1})$. At the same time the critical area $s_m = s_\alpha(q_m)$ is minimal for square contours. Thus, all configurations containing contours with $s_\alpha \geqq s_{mm} = q_{mm}^d$ should be excluded, because they do not correspond to the metastable state but describe a stable or a decaying state.

The restricted partition function Z_p^{+*}, containing all the contours with $s_\alpha < s_{mm}$ (s_{mm} is now arbitrary fixed) has the following properties. The pressure $F_p^* = S_p^{-1} \ln Z_p^{+*}$ has the thermodynamic limit $F_p^* \to F^*$ for $h < 0$, because F_p^* is bounded and increases, when $p \to \infty$. According to Theorem 1, $Z_p^{+*} \neq 0$ in the circle $|h| < r_m = 2dEs_{mm}^{-1/d}/(1 + C_2^{-1})$, and thus F_p^* has a thermodynamic limit F^* in this circle. The point h_0 corresponding to s_{mm} is $h_0 = 2(d-1)Es_{mm}^{-1/d}$. Therefore h_0 is in this circle and F^* can be calculated with the help of the expansion $F^*(h_0) = F^*(0) + [F^*]^{(1)} h_0/1! + [F^*]^{(2)} h_0^2/2! + \ldots$ (this series converges).

In fact the picture is more complicated. We cannot separate all the contours strictly into two classes, containing respectively large and small contours. A group of intermediate nearly-critical contours with $s_\alpha \sim s_{mm}$, $l_\alpha \sim l_{mm}$ exists. Now two different results are possible when such contours appear: the system can pass into the stable state or remain in the metastable one. As a consequence, we can calculate $F^*(h, E)$ only with an uncertainty $\delta = \delta(h, E)$. A lower bound for δ may be derived if we consider that the group of intermediate contours contains only one square contour with $s_\alpha = q_{mm}^d$. In this case $\delta_{\min} = P_{mm}(h, E)$. An upper bound is $\delta_{\max} = P_{mm}(h, E - \ln C_1)$, because the number of contours in the intermediate group is less than $C_1^{l_{mm}}$.

Concerning the main result, we have already remarked that the expansion $F^+(h) \sim A_0 + A_1 h + A_2 h^2 + \ldots$ does not converge. We can try to calculate $F(h)$ using this asymptotic expansion, but the values of $F(h)$ will be obtained with the uncertainty $\varepsilon = \varepsilon(h)$ common for all asymptotic expansions. The sequence $A_k h^k$ attains its minimum for $k = k_m$, $k_m = (2(d-1)(E + \xi C))^d / h^{d-1}$, and simple calculations give $\varepsilon = \exp(-2^d (E + \xi C)^d ((d-1)/h)^{d-1})$ (we suppose that $\varepsilon = A_{k_m} h^{k_m}$).

Thus, $\varepsilon = P_{mm}(h, E+\xi C)$ so that ε is equal to the physical uncertainty δ and we cannot consider this result as an accidental one. We conclude that the system, being in the stable state, feels both the transition and the instability in the metastable phase since the coefficients A_k have been obtained from the stable phase $(h<0)$.

Finally one may suppose that the main properties of the first order phase transition proved for the Ising model remain true for a wider class of lattice and continuous models. Namely, the point of the phase transition is a point of non-analyticity of the thermodynamic functions. The asymptotic expansion gives a correct result for the metastable phase with the uncertainty ε equal to the physical uncertainty δ. Analytic continuation in the point of the phase transition becomes possible as soon as we forbid the decay of the system into the stable phase by means of some mathematical restrictions or by any external physical forces.

Appendix

Proof of Theorem 3. The coefficient a_k can be calculated by using the Cauchy formula:

$$a_k = \frac{1}{\pi r^k} \int_0^{\pi} e^{r\cos\varphi + \mathrm{Re} f(z)} \cos\psi(\varphi)\, d\varphi\,, \tag{A.1}$$

when the contour of integration is the circle $z = r e^{i\varphi}$ $(0<r<R)$. Here $\psi(\varphi) = r\sin\varphi + \mathrm{Im} f(z) - k\varphi$, and the equality $f^*(z) = f(z^*)$ is used. The parameter r will be fixed later. The derivatives of $f(z)$

$$\frac{df}{d\varphi} = izf'\,, \quad \frac{d^2f}{d\varphi^2} = -zf' - z^2f''\,, \quad \frac{d^3f}{d\varphi^3} = -izf' - 3iz^2f'' - iz^3f'''\,,$$

$\left(\frac{dz}{d\varphi} = iz\right)$ enable us to obtain

$$\mathrm{Re} f(z) = f(r) + \frac{\varphi^2}{2}\mathrm{Re}\frac{d^2f}{d\varphi^2}_{|\varphi=\varphi'} \qquad (0<\varphi'<\varphi)\,, \tag{A.2}$$

$$\mathrm{Im} f(z) = rf'(r)\varphi + \frac{\varphi^3}{6}\mathrm{Im}\frac{d^3f}{d\varphi^3}_{|\varphi=\varphi'} \qquad (0<\varphi'<\varphi)\,. \tag{A.3}$$

The point $z = r e^{i\varphi}$ for an arbitrary φ is situated at a distance $R-r$ from the circle $|z| = R$, inside which $f(z)$ is an analytic function. Thus we get

$$|f'(z)| < A\,, \quad |f''(z)| < A/(R-r)\,, \quad |f'''(z)| < 2A/(R-r)^2\,.$$

Upper bounds for the last terms in (A.2) and (A.3) are then obtained:

$$\left|\mathrm{Re}\frac{d^2f}{d\varphi^2}\right| \leqq \left|\frac{d^2f}{d\varphi^2}\right| \leqq r|f'| + r^2|f''| < ArR/(R-r)\,, \tag{A.4}$$

$$\left|\mathrm{Im}\frac{d^3f}{d\varphi^3}\right| \leqq r^3|f'''| + 3r^2|f''| + r|f'| < ArR(R+r)/(R-r)^2\,. \tag{A.5}$$

Moreover,

$$\psi(\varphi)=r\varphi+rf'(r)\varphi-k\varphi+\frac{\varphi^3}{6}\left(\frac{ArR(R+r)}{(R-r)^2}+r\right)\xi\,, \tag{A.6}$$

where we have used $\sin\varphi=\varphi+\varphi^3\xi_1/6$, $(-1\leqq\xi_1\leqq 1)$.

Equation (2.8) has a solution for $0<r<R$, because, when r changes from 0 to R, the left side of the equation changes from 0 to $R(1+f'(R))$ and $R(1+f'(R)) >R(1-A)>R(1-2\sqrt{A})>k$, $(|f'|\leqq A<1/4)$. Taking r as a solution of Eq. (2.8), the first three terms vanish in (A.6).

From the conditions $R(1-2\sqrt{A})>k$, $r(1+f'(r))=k$ and $|f'|\leqq A$ we obtain $R(1-2\sqrt{A})>r(1-A)$ and $\delta<(1-2\sqrt{A})/(1-A)$, where $\delta=r/R$. Then the inequatilies

$$AR/(R-r)<A(1-A)/(2\sqrt{A}-A)<1/4\,, \tag{A.7}$$

$$AR(R+r)/(R-r)^2<(2-2\sqrt{A}-A)(1-A)/(2-\sqrt{A})^2<1 \tag{A.8}$$

lead to the estimates $\left|\mathrm{Re}\dfrac{d^2f}{d\varphi^2}\right|<r/4$, $|\psi(\varphi)|<\varphi^3r/3$.

Now we derive the upper bound for a_k. From Eq. (A.1) we get

$$a_k<\frac{1}{\pi r^k}e^{r+f(r)}\int_0^\pi \exp(-r(1-\cos\varphi-\varphi^2/8))d\varphi \tag{A.9}$$

$(\cos\psi<1$, $\mathrm{Re}f(z)<f(r)+\varphi^2r/8)$. Inequality $r>80$ follows from $(1+f'(r))=k$, $k>100$ and $|f'|<1/4$. The integral in (A.9) has a limit $\sqrt{2\pi/3r}$ when $r\to\infty$, and simple calculations for $r>80$ show that the integral is less than $\pi/\sqrt{r}$. Thus the upper bound (2.7) is proved.

To prove the lower bound we divide the region $0<\varphi<\pi$ into two parts: $0<\varphi<\gamma$ and $\gamma<\varphi<\pi$, where $\gamma=(3/r)^{1/3}$. The corresponding integrals will be denoted by I_1 and I_2:

$$I_1=\int_0^\gamma e^{r\cos\varphi+\mathrm{Re}f}\cos\psi\,d\varphi\,.$$

It is easy to see that $\psi<1$ and $\cos\psi>1/2$ for $0<\varphi<\gamma$. Thus we have

$$I_1>\frac{1}{2}e^{r+f(r)}\int_0^\gamma \exp\left(-\frac{5}{8}r\varphi^2\right)d\varphi=e^{r+f(r)}\sqrt{\frac{2}{5r}}\int_0^x e^{-t^2}dt>\frac{\pi}{6\sqrt{r}}e^{r+f(r)}\,. \tag{A.10}$$

Here we used $x=\sqrt{5r/8}\gamma=r^{1/6}(5/8)^{1/2}3^{1/3}$ and $\cos\varphi\geqq 1-\varphi^2/2$, $\mathrm{Re}f >f(r)-\varphi^2r/8$. Now it is sufficient to obtain an upper bound for I_2:

$$|I_2|<e^{r+f(r)}\int_\gamma^\pi \exp(-r(1-\cos\varphi-\varphi^2/8))d\varphi\,.$$

The last integral is of the order of $\exp(-r^{1/3})$ for large r, because γ is of the order of $r^{-1/3}$. Calculations for $r>80$ give the estimate $|I_2|<\pi e^{r+f(r)}/12\sqrt{r}$. The first inequality in (2.7) follows from this estimate and (A.10).

Finally we prove the uniqueness of the solution r. If r is a solution of Eq. (2.8), the derivative $\frac{d}{dr}r(1+f'(r))$ is positive: $(r(1+f'(r)))'=1+f'(r)+rf''(r) > 1-A-rA/(R-r)=1-A/(1-\delta)>0$. That makes the existence of two or more solutions impossible.

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