EXISTENCE OF PHASE TRANSITIONS IN MODELS OF A LATTICE GAS

R. L. DOBRUSHIN
UNIVERSITY OF MOSCOW

1. Introduction

It is proved here that at sufficiently low temperatures, a phase transition occurs in the model of a lattice gas with pairwise interaction of the particles, if a constraint, meaning roughly that the negative part of the potential in some sense "outweighs" its positive part, is imposed on the interaction potential; or if the potential is nonzero, nonpositive, and decreases sufficiently rapidly at infinity. The proof is based on a further development of the method introduced independently by the author in [1], [2] for the proof of the existence of a phase transition in the Ising model of a lattice gas, and by Griffiths [3] for the solution of a similar problem. Using the same method, Berezin and Sinai [4] proved the existence of a phase transition in models of a lattice gas with a nonpositive finite potential, which is negative in the segment $[0, R]$.

All the constructions presented below are carried out analogously for lattices of any dimensionality greater than one (as is known, there are no phase transitions in one-dimensional lattices). For greater clarity, we carry out the reasoning for two-dimensional lattices (the generalization to higher dimensions is described in detail in [2]).

Let V_ℓ be a square with side ℓ in a two-dimensional square lattice, that is, the set of points $X = (x_1, x_2)$, $x_i = 1, 2, \cdots, \ell$; $i = 1, 2$. We shall call the subset $a = (X_1, \cdots, X_N)$ of N elements of V_ℓ the *arrangement* of N particles in the square V_ℓ. We denote the set of all such arrangements by $\mathcal{V}_{N,\ell}$. For clarity, we shall often interpret V_ℓ as a square piece of graph paper with unit square cells by assigning to the point of the lattice a cell whose center is this point. The arrangement a is thereby interpreted as a way of choosing N of the ℓ^2 cells in V_ℓ, which are declared *filled*, while the rest, including the cells outside V_ℓ, are *empty*. The *potential* will be a function $U(Y)$ defined in the set R of all integer, two-dimensional vectors Y, except zero, and depending only on the length $|Y|$ of the vector Y. (The results extend almost without change to the case in which $U(Y)$ can depend on the direction of Y.) The number

$$Z(N, \ell, T) = \sum_{a \in \mathcal{V}_{N,\ell}} \exp\left\{-\frac{1}{T}\sum_{i<j} U(X_i - X_j)\right\} \tag{1.1}$$

is called the statistical sum. The constant $T > 0$ is the gas *temperature*. Suppose that

$$(1.2)\qquad |U(Y)| \leq C|Y|^{-2-\epsilon}$$

for some $C < \infty$ and some $\epsilon > 0$. Under the assumption that the number of particles N_ℓ depends on ℓ and that

$$(1.3)\qquad \lim_{\ell \to \infty} \frac{\ell^2}{N_\ell} = v = \frac{1}{\lambda}, \qquad 1 < v < \infty$$

(v is called the *specific volume,* and λ is the *particle density*), there exists a finite limit

$$(1.4)\qquad f(v, T) = \lim_{\ell \to \infty} \frac{1}{N_\ell} \log Z(N_\ell, \ell, T)$$

where $f(v, T)$ is a convex, continuous function of v for any fixed T. The proof of the analogous fact for a continuous model (see [5]) carries over literally to the lattice case considered here. It has been shown in [5] that although condition (1.2) may be weakened slightly, it is impossible to set $\epsilon = 0$ in it.

The segment $[v_1, v_2]$, $v_1 < v_2$ is called a *phase-transition segment* for some fixed T if $f(v, T)$ is for this T, a linear function of v for $v_1 \leq v \leq v_2$. Physically this means that the gas *pressure,* equal to $T(\partial f(v, t)/\partial v)$, and its *chemical* potential $T(v(\partial f(v, T)/\partial v) - f(v, T))$ are constant in the phase-transition segment.

THEOREM. *Let E_i, $i = 1, 2, 3, 4$, be integer vectors of unit length and let $\mathfrak{D} \subset R$ be the set of vectors Y such that $U(Y) > 0$. Let $\bar{\mathfrak{D}}$ be the complement of $\mathfrak{D}$. Assume that the following conditions are satisfied:* (1) *either the inequality*

$$(1.5)\qquad \sum_{Y \in \mathfrak{D}} (|Y| + 1)\, U(Y)$$
$$< -\tfrac{1}{4} \sum_{Y \in \bar{\mathfrak{D}}, Y + E_1 \in \bar{\mathfrak{D}}, \cdots, Y + E_4 \in \bar{\mathfrak{D}}} \max\,(U(Y), U(Y + E_1), \cdots, U(Y + E_4))$$

holds, or $\mathfrak{D}$ is empty and $U(Y)$ is not identically zero; and (2) *there exist constants $C < \infty$ and $\epsilon > 0$ such that*

$$(1.6)\qquad |U(Y)| \leq C|Y|^{-4-\epsilon}.$$

Then there exists a $T_{cr} > 0$ such that for $T < T_{cr}$ there is a nonempty phase-transition segment $[v_1^T, v_2^T]$. As $T \to 0$ the limits of the segment are $v_1^T \to 1$, $v_2^T \to \infty$.

(In the three-dimensional case, it is necessary to replace 4 by 6 in (1.6), and the factor $\frac{1}{4}$ by $\frac{1}{9}$ in (1.5).)

Let us note that for condition (1.5) of the theorem to be satisfied it is sufficient that the set $\mathfrak{D}$ lie in a circle of radius R_0, that the inequality

$$(1.7)\qquad U(Y) \leq -B, \qquad B > 0, \qquad R_1 < |Y| < R_2$$

be satisfied in the segment $[R_1, R_2]$, and that

$$(1.8)\qquad (R_0 + 2)^3 \max U(Y) < \tfrac{1}{4} B[(R_2 - 3)^2 - (R_1 + 3)^2].$$

This follows from the fact that $\pi(R_0 + 2)^2$ and $\pi[(R_2 - 3)^2 - (R_1 + 3)^2]$ are, respectively, upper and lower bounds for the number of integer vectors in the circle of radius R_0 and in the annulus between the circles of radii $R_1 + 1$ and $R_2 - 1$. Therefore, condition (1.5) is an explicit form of the assumption that the negative part of the potential "outweighs" the positive part. The specific form of this condition is associated mainly with the method of proof proposed here, and it has no independent physical meaning. Even without introducing new ideas into the arguments it could be weakened somewhat, but at the expense of complicating its formulation. On the other hand, there are intuitive grounds for considering that some condition of a similar type is necessary for the existence of the phase transition of the kind considered here. As regards condition (1.6), it is not different in principle from the optimum condition (1.2), and is introduced to facilitate the proofs.

We shall not give estimates for T_{cr} and v_1^T, v_2^T, which could be obtained by retracing the subsequent proofs since they would be very rough for nowhere in the course of the arguments did the question of their refinement arise. Only one among all the physical constants associated with the phase transition was calculated. We shall show that the chemical potential at the phase-transition point is equal to the value μ, given by

$$\mu = \tfrac{1}{2} \sum_{Y \in R} U(Y). \tag{1.9}$$

The series giving the right side of this equality will converge because of the inequality (1.6).

2. A probabilistic lemma

Let $\mathcal{V}_\ell = \bigcup_{N=0}^{\ell^2} \mathcal{V}_{N,\ell}$ be the set of arrangements having arbitrary numbers of particles in V_ℓ. It will later be convenient to consider the arrangement $a \in \mathcal{V}$ as a function G_Y, where the argument Y runs over all possible two-dimensional integer vectors, and the value $G_Y = 1$ is taken, if a particle is at a point corresponding to Y (the corresponding cell is filled), and $G_Y = 0$ if no particle is there (the corresponding cell is empty; all the cells outside V_ℓ are empty). Let $N(a)$, $a \in \mathcal{V}_\ell$ denote the number of particles for the arrangement a (the number of filled cells).

Let us now introduce the function

$$W(a) = -\tfrac{1}{2} \sum_{GY_1 = 1, GY_2 = 0} U(Y_1 - Y_2). \tag{2.1}$$

(The summation in (2.1) extends over the set of pairs of cells, one of which is occupied, and the other is empty.) Evidently, for $a = (G_Y, Y \in R) = (X_1, \cdots, X_N)$,

$$\begin{aligned} W(a) &= -\tfrac{1}{2} \sum_{GY_1 = 1, Y_2 \neq Y_1} U(Y_1 - Y_2) + \tfrac{1}{2} \sum_{GY_1 = 1, GY_2 = 1, Y_2 \neq Y_1} U(Y_1 - Y_2) \\ &= -\mu N(a) + \sum_{i<j} U(X_i - X_j). \end{aligned} \tag{2.2}$$

Finally, let us consider the probability distribution in $\mathcal{V}_\ell$ given for $S \subset \mathcal{V}_\ell$ by the formula

$$\Pr_\ell \{S\} = Q(\ell)^{-1} \sum_{a \in S} \exp\left\{-\frac{1}{T} W(a)\right\}, \tag{2.3}$$

with the normalizing factor

$$Q(\ell) = \sum_{a \in \mathcal{V}_\ell} \exp\left\{-\frac{1}{T} W(a)\right\}. \tag{2.4}$$

(The dependence of $Q(\ell)$ on T will not be indicated explicitly in this notation.) In conformity with (2.2), the distribution (2.3) may be interpreted in physical language as the distribution in a large canonical ensemble with the chemical potential μ.

LEMMA 1. *In order that a nonempty phase-transition segment with chemical potential* μ, *given by* (1.9), *exist for some* T, *it is sufficient that for some* $\delta > 0$, $\gamma > 0$ *and all sufficiently large* ℓ,

$$\Pr_\ell\left\{\left|\frac{N(a)}{\ell^2} - \tfrac{1}{2}\right| \geq \delta\right\} > \gamma. \tag{2.5}$$

The segment $[(\frac{1}{2} + \delta)^{-1}, (\frac{1}{2} - \delta)^{-1}]$ *is in this case a phase-transition segment.*

The proof presented below also shows that the necessary and sufficient condition for a phase transition with chemical potential μ is that the left side in (2.5) should not approach zero exponentially rapidly as $\ell \to \infty$.

PROOF. It follows from (2.2), (2.3), and (2.4) that

$$\Pr_\ell\left\{\left|\frac{N(a)}{\ell^2} - \tfrac{1}{2}\right| \geq \delta\right\} = \left(\sum_{|N - \frac{1}{2}\ell^2| \geq \delta\ell^2} Q(N, \ell)\right)\left(\sum_{N=0}^{\ell^2} Q(N, \ell)\right)^{-1} \tag{2.6}$$

where

$$Q(N, \ell) = Z(N, \ell, T) \exp\left\{\frac{\mu}{T} N\right\} = \sum_{N(a) = N} \exp\left\{-\tfrac{1}{2} W(a)\right\}. \tag{2.7}$$

Furthermore, taking into account condition (1.3), we deduce from (1.4) that

$$\lim_{\ell \to \omega} \frac{1}{\ell^2} \log Q(N_\ell, \ell) = \frac{\mu\lambda}{T} + \lambda f\left(\frac{1}{\lambda}, T\right) = g(\lambda, T). \tag{2.8}$$

From the fact that $f(v, T)$ is a convex continuous function of v, it follows that $g(\lambda, T)$ is a convex continuous function of λ (this can be proved, for instance, by differentiation). Moreover, let us show that

$$g(\tfrac{1}{2} - \delta, T) = g(\tfrac{1}{2} + \delta, T). \tag{2.9}$$

Indeed, let us consider the arrangement $\bar{a} \in \mathcal{V}_\ell$, which is obtained from the arrangement $a \in \mathcal{V}_\ell$ if the empty cells in V_ℓ are replaced by filled cells, and the filled cells by empty cells (the cells outside V_ℓ do not change). With this definition one can write (see (2.1))

$$\begin{aligned} W(a) - W(\bar{a}) \\ = +\tfrac{1}{2} \sum_{G_{Y_1}=0, Y_2 \notin V_\ell, Y_1 \in V_\ell} U(Y_1 - Y_2) - \tfrac{1}{2} \sum_{G_{Y_1}=1, Y_2 \notin V_\ell} U(Y_1 - Y_2). \end{aligned} \tag{2.10}$$

Because of the absolute convergence of the series (1.9), for any $\epsilon > 0$ there exists an $R < \infty$ such that as soon as the distance from Y_1 to the boundary of the square V_ℓ exceeds R, then $\frac{1}{2} \sum_{Y_2 \notin V_\ell} |U(Y_1 - Y_2)| < \epsilon$. It follows that as

$\ell \to \infty$ the difference $W(\bar{a}) - W(a)$ is of the order of magnitude $o(\ell^2)$ uniformly in a. Finally, since the correspondence between a and $\bar{a}$ is one-to-one, and since $N(\bar{a}) = \ell^2 - N(a)$, then, according to (2.7),

$$(2.11) \qquad Q(N, \ell) = Q(\ell^2 - N, \ell) \exp\{o(\ell^2)\}$$

from which (2.9) follows.

Using the estimates

$$\max_{|N - \frac{1}{2}\ell^2| \geq \delta\ell^2} Q(N, \ell) \leq \sum_{|N - \frac{1}{2}\ell^2| \geq \delta\ell^2} Q(N, \ell) \leq \ell^2 \max_{|N - \frac{1}{2}\ell^2| \geq \delta\ell^2} Q(N, \ell),$$

$$(2.12) \qquad Q(N, \ell) \leq C_{\ell^2}^N \exp\left\{\frac{N}{2T} \sum_Y |U(Y)|\right\}$$
$$\leq \left(\frac{\ell^2}{N}\right)^N \ell^N \exp\left\{\frac{N}{2T} \sum_Y |U(Y)|\right\} \leq \exp\{\ell^2 \varphi(N/\ell^2)\}$$

where $\varphi(x) \to 0$ as $x \to 0$, and the inequality $g(\lambda, T) \geq 0$ we find from (2.6) and (2.7) that

$$(2.13) \qquad \lim_{\ell \to \infty} \frac{1}{\ell^2} \log \Pr_\ell \left\{\left|\frac{N(a)}{\ell^2} - \tfrac{1}{2}\right| \geq \delta\right\}$$
$$= \max_{|\lambda - \frac{1}{2}| \geq \delta} g(\lambda, T) - \max_{0 \leq \lambda \leq 1} g(\lambda, T) = g(\tfrac{1}{2} - \delta) - g(\tfrac{1}{2}).$$

The convexity and symmetry of $g(\lambda, T)$ are used in the last equality. Since it follows from (2.5) that the right side in (2.13) is zero, then under the conditions of the lemma, $g(\lambda, T)$ is constant in the segment $[\frac{1}{2} - \delta, \frac{1}{2} + \delta]$. It now follows from (2.8) that for $v \in [(\frac{1}{2} + \delta)^{-1}, (\frac{1}{2} - \delta)^{-1}]$,

$$(2.14) \qquad f(v, T) = vg(\tfrac{1}{2}, T) - \frac{\mu}{T}$$

and the statement of the lemma now follows from the definition of the phase transition and the chemical potential.

Lemma 1 is due to Berezin and Sinai [4]; however, the proof they proposed is more complicated than the one presented above. This lemma reduces the question of the phase transition to the question of "violation of the law of large numbers" in a large canonical ensemble (inequality (2.5)). The purpose of Griffiths' work [3] was the deduction of the fact that for sufficiently large T and ℓ the mean value of $N(a)/\ell^2$ is less than $\frac{1}{2} - \delta$, from which (2.5) certainly results. In [2] the author used a stronger condition of the same kind rather than the equality (2.5) as the sufficient condition for a phase transition, and this led to the introduction of complicated constructions now shown to be unnecessary. However, they appear to have independent interest.

3. The tree of connected components

Let us take some number $M > 0$, whose exact value will be chosen below. Without restricting the generality, we may consider only values of ℓ which are multiples of M. With this choice of M the square V_ℓ is divided into $(\ell/M)^2$ subsquares containing M^2 cells each. We call these subsquares *boxes.*

Moreover, let us consider a fixed arrangement a in V_ℓ. Let us call a box a *box with filler* (respectively, a *box with emptiness*) if it contains at least one filled (respectively empty) cell. Each box is either with emptiness or with filler, but these two possibilities are not exclusive. The boxes outside V_ℓ are boxes with emptiness, but without filler. We call two boxes *contiguous* if they have a common side or vertex. Call *path* a finite sequence of boxes in which the adjoining boxes in the sequence are contiguous. A subset of boxes such that for any two boxes of the subset there is from one to the other a path composed of boxes of this subset will be called a connected set. A set of boxes with a filler decomposes uniquely into connected components which we call *components of boxes with a filler. Components of boxes with emptiness* are defined analogously. Among the components there is exactly one component of boxes with emptiness which contains the exterior of V_ℓ. It will be called the *initial component.* We call two components *contiguous* if they contain a common box or two contiguous boxes. Evidently only a component with filler and a component with emptiness may be contiguous.

LEMMA 2. *If the components are interpreted as the vertices of a graph, and the contiguous components are connected by links, then this graph turns out to be a tree, that is, the graph has no cycles. Its vertex is the initial component.*

PROOF. Geometrically it is evident that to each finite connected set of boxes there corresponds uniquely a closed broken line which does not reintersect itself (double return to one vertex is permitted) and is such that the whole set lies within this broken line, with a box from the set on the inside of each link and a box from the complement on the outside of the link. We will call such a broken line associated with a component the *envelope of the component.* Only the initial component has no envelope. Let a component A, for definiteness be a component with filler. Then all the boxes adjoining its envelope from outside its links will belong to the same component with emptiness. They may be connected by a path along the envelope. We denote this component by $\bar{A}$ and we call it the *enclosure of the component A*. Evidently $\bar{A}$ is contiguous to A. We call the component B *external* (correspondingly *internal*) to A if it is not an enclosure of A and consists only of boxes external (internal) with respect to the envelope of A. Let us show that there are only four possibilities.

Component B may be either an enclosure, or external, or internal to A, or may coincide with A. In fact, since any path of boxes connecting the boxes within and without the envelope "intersects" the envelope, and hence, has common boxes with A and $\bar{A}$, then component B, which is not external or internal, coincides with A or $\bar{A}$. Moreover, let us show that if the component A is contiguous to another component B, then either A is the enclosure of B or B is the enclosure of A. Indeed, let us note that if one component is external to another, these components may not be contiguous. Hence, if the statement were not true, then A would turn out to be a component internal for B, and B

would be internal for A. Then these two different components would have a common envelope, which is impossible.

Turning directly to the proof of the lemma, let us assume that there is a sequence of components $A_1, A_2, \cdots, A_n = A_1$ such that A_i is contiguous to A_{i+1}. Since for each component there is only one component which is the enclosure of it, either each next component in this sequence is the enclosure of the preceding, or conversely, each preceding component is the enclosure of the next. But evidently if A is the enclosure of B, then the envelope of B will lie within the envelope for A. And if the statement of the lemma were false, we would have a cyclic sequence of plane broken lines lying within each other, which is impossible according to topological considerations. Since only the initial component has no envelope, it is the vertex of the tree.

Let us call the subset of boxes from A, which are also boxes from B or are contiguous to boxes from B, the boundary between components A and B.

LEMMA 3. *For any components A and B the boundary between A and B is a connected set of boxes.*

PROOF. Since the boundary is empty for noncontiguous components, then without limiting the generality it may be assumed that A is a component with filler, and B is a component with emptiness. Let a and $\tilde{a}$ be arbitrary boxes from A on the boundary with B. Let b and $\tilde{b}$ be boxes from B contiguous to a and $\tilde{a}$, respectively. There exists a path α from a to $\tilde{a}$, which lies in A, and a path β from B to $\tilde{b}$, lying in B, since the components A and B are connected. It is necessary to construct a path γ from a to $\tilde{a}$, which will lie on the boundary between A and B. We shall later interpret the path as a broken line whose links connect the centers of adjacent boxes of the path. Since the path γ may be constructed successively from one point of intersection of the paths α and β to their next point of intersection, then we assume without restricting the generality, that the paths α and β do not intersect (except possibly at the endpoints). Appending segments connecting a to b and $\tilde{a}$ to $\tilde{b}$ to α and β, we obtain a closed contour within which a set of boxes C lies. The intersection $A \cap C$ decomposes into connected components, one of which $\tilde{A}$ abuts on the path α. The envelope of $\tilde{A}$ (defined in exactly the same way as the envelope of the component in the proof of lemma 2) consists of γ and of a second path δ which also goes from a to $\tilde{a}$. A path going from b to $\tilde{b}$ can be drawn along the boxes with emptiness adjacent to the boxes from δ. Hence, these adjacent boxes belong to B. This means that the boxes in δ lie on the boundary between A and B, and δ is the desired path.

4. A bound on the number of ways of producing a given arrangement

Let us number the boxes from V_ℓ in some way by numbers $1, \cdots, (\ell/M)^2$. Let us ascribe to each component, except the initial component, a number equal to the smallest of the numbers of the boxes of the outside boundary of this component. The numbers may take the values $1, \cdots, (\ell/M)^2$, but not all of them correspond to a component. We shall consider that each filled cell from V_ℓ belongs to a component of boxes with filler, which contains the box in which this cell lies. We proceed analogously with the empty cells. Let us designate the component B as *upper relative to the component* A if the path of components from B along branches of the tree to the vertex of the tree does not pass through A. All the remaining components (including component A itself) will be called lower *relative* to A. Define a mapping $T_i(a)$, $i = 1, \cdots, (\ell/M)^2$ transforming all the arrangements $\mathcal{V}_\ell$ into $\mathcal{V}_\ell$ as follows. If there are no components with number i in the arrangement a, then $T_i(a) = a$. If A_i is the component with number i in the arrangement a, then in constructing $T_i(a)$ by means of a for all cells belonging to the components of the arrangement a which are lower relative to A_i, the filled cells are replaced by the empty cells, and the empty by the filled; the cells of components which are upper relative to A_i remain unchanged.

Let us designate the boundary with the adjacent upper component as the *upper boundary* of the component A_i. Let $K_i(a)$ be *the number of boxes belonging to the upper boundary of the component.* The component A_i does not exist, let $K_i(a) = 0$.

LEMMA 4. *There exists a constant* $\mathfrak{D} < \infty$ *such that for any* $i = 1, \cdots, (l/m)^2$ *and any* $a \in \mathcal{V}_\ell$ *the number of arrangements* $\tilde{a} \in \mathcal{V}_\ell$ *such that* $T_i(a) = T_i(\tilde{a})$, *does not exceed* $\mathfrak{D}^{K_i(a)}$.

PROOF. Let us prove, first, that the quantity of different connected sets of K boxes which have a common box does not exceed 7^K. Indeed, each box has eight sides and vertices which we number $1, \cdots, 8$. Furthermore, let us introduce the following method of numbering boxes of any of the sets under consideration by the numbers $1, 2, \cdots, K$. If the numbers $1, \cdots, i$ have already been ascribed to boxes, we then select the least, in number, of the numbered boxes to whose side or vertex a still unnumbered box of the set adjoins; we select that one of these adjoining unnumbered boxes which adjoins the side or the vertex with the least number and we ascribe the number $i + 1$ to this chosen box. By virtue of connectedness, any box of the set receives a number. Let us note now that even if the set were not known in advance, the numbering possibilities at each step of our algarithm, except the first and second, will not be greater than the seven possibilities of selecting the box next in number; at the second step it will be eight, and at the first, one. Hence, it also follows that the number of sets considered is not greater than $8 \cdot 7^{K-2} < 7^K$.

Having fixed the arrangement a and the component A_i, let us call a box *upper* if it belongs to a component which is upper relative to A_i. We define a lower box analogously. If the box belongs to two components at once, then these components are adjacent. Hence, only boxes of the outer boundary of A_i may be simultaneously upper and lower; that is, boxes are classified in three groups: upper, lower, and belonging to the outer boundary. The mapping $T_i(a)$ may now be described thusly: the arrangement in the upper boxes remains unchanged; the filled cells in the lower boxes are replaced by empty ones, and the empty ones by filled; the box of the outer boundary becomes entirely empty if A_i is a component of boxes with filler, and becomes entirely filled if A_i is a component of boxes with emptiness. Furthermore, it may be asserted that a box is upper if and only if from any other upper box there exists leading to it a path which does not also pass through the outer boundary of A_i. This easily follows from the fact that a path along the tree of components passing successively over the components to which these boxes belong may be associated with any other along the boxes; and conversely, for any path along the tree of components it is possible to construct a path along the boxes which will run through the boxes of these components in sequence.

From the description just given of upper boxes it results that their set is uniquely determined, for given a and A_i, if the boxes of the outer boundary are specified. Therefore, the total number of different methods of classifying all the boxes into upper, lower, and boxes of the outer boundary equals the number of methods of selecting boxes of the outer boundary; and this number, by virtue of lemma 3 on the connectedness of the boundary and the estimate given above, does not exceed $7^{K_i(a)}$ (for all a the components of A_i have a common box with number i). Knowing which boxes are upper and which are lower for the arrangement a, we may reproduce the arrangement in these boxes by means of $T_i(a)$. Since the arrangement in any box may be given by 2^{M^2} different methods, the number of different ways of reproducing the arrangement a in the boxes of the outer boundary of A_i by means of $T_i(a)$ is $2^{M^2K_i(a)}$, and we obtain that the total number of methods of reproducing a by means of $T_i(a)$ does not exceed $(7.2^{M^2})^{K_i(a)}$, and lemma 4 is proved for $\mathfrak{D} = 7.2^{M^2}$.

5. An estimate of the function W(a)

Let us call the potential $U(Y)$ *nonperiodic* if there exists a finite sequence of vectors $\overline{Y}_1, \cdots, \overline{Y}_m$ such that $U(\overline{Y}_i) \neq 0$, $i = 1, \cdots, m$, and $\overline{Y}_1 = \overline{Y}_2 + \cdots + \overline{Y}_m = E$, where E is the unit vector.

LEMMA 5. *If inequality* (1.5) *is true or if the potential* $U(Y)$ *is a nonpositive, nonperiodic potential, and if, in addition* (1.6) *is true, then one may choose the length* M *of the side of the box in such a way that there is a constant* $d > 0$ *such that for any* $a \in \mathcal{V}_\ell$, $i = 1, \cdots, (\ell/M)^2$, *the inequality*

$$W(a) - W(T_i(a)) \geq dK_i(a) \tag{5.1}$$

holds.

PROOF. In conformity with definition (2.1) and the definition of the transformation $T_i(a)$, either the term $-\frac{1}{2}\, U(Y_1 - Y_2)$ enters simultaneously in both the sums defining $W(a)$ and $W(T_i(a))$, or it does not enter in either of these sums if both cells Y_1, Y_2, belong to the upper component relative to A_i or both belong to the lower component relative to A_i. On the other hand, let one of the cells Y_1, Y_2 belong to the upper and the other to the lower component. If one of these cells is filled, and the other is empty, then $-\frac{1}{2}\, U(Y_1 - Y_2)$ enters into the sum for a, but it does not enter into the sum for $T_i(a)$. Conversely, if both these cells are filled or both are empty, then $-\frac{1}{2}U(Y_1 - Y_2)$ does not enter into the sum for a, but it enters into the sum for $T_i(a)$. Hence, if F is the set of upper and $\overline{F}$ the set of lower cells, then

$$W(a) - W(T_i(a)) = \frac{1}{2} \sum_{Y_1 \in \overline{F}, Y_2 \in F} \gamma_{Y_1,Y_2} U(Y_1 - Y_2) \tag{5.2}$$

where $\gamma_{Y_1,Y_2} = -1$, if one of the cells Y_1, Y_2 is filled and the other is empty, and $\gamma_{Y_1,Y_2} = 1$ otherwise.

Later we shall consider several particular cases in turn. Let us assume first that $U(Y)$ is a nonperiodic, nonpositive, finite potential (that is, U vanishes for $|Y| > R$, $R < \infty$). Let us select M so that $M > R$ and so that all the terms $\overline{Y}_i$ and all the partial sums $\overline{Y}_1 + \overline{Y}_2 + \cdots + \overline{Y}_i$, $i = 1, \cdots, m$ in the sequence defining the nonperiodicity of the potential, are less than M in absolute value. Let us note first that because of the finiteness condition $U(Y_1 - Y_2) \neq 0$ only if Y_1 and Y_2 belong to the same or adjoining boxes. But if both cells Y_1 and Y_2 are empty here, or both are filled, then they belong to the same component and the corresponding term does not enter into (5.2). This means there are no terms with $\gamma_{Y_1,Y_2} = 1$ in (5.2), and $W(a) \geq W(T_i(a))$ in the case under consideration. In order to give a more exact estimate of the type (5.1), let us note that if some box belongs to the outer boundary of A_i, that is, the boundary of A_i with the component $\overline{A}$ which is upper and adjacent to A_i, then there is a cell Y appearing in A_i which is in this box or in the adjacent box belonging to the outer boundary, such that the cell $Y + E$ (where E is any unit vector) belongs to $\overline{A}$. Indeed, this is obvious if the box b belongs to A_i and $\overline{A}$ simultaneously, and hence contains both the cells entering in A_i and those entering in $\overline{A}$. Therefore, this is true even if one of the adjacent boxes b belongs to A_i and $\overline{A}$ simultaneously. Finally, if the box b belongs only to A_i, and the adjacent boxes only to $\overline{A}$, then the cells abutting on the sides of the box b possess the required property. Furthermore, let Y belong to A_i and $Y + E$ to $\overline{A}$. Let us consider the sequence of cells $Y, Y + \overline{Y}_1, \cdots, Y + \overline{Y}_1 + \cdots + \overline{Y}_m + Y + E$. In conformity with the selection of M, the neighboring terms of this sequence $Y + \overline{Y}_1 + \cdots + \overline{Y}_i$ and $Y + \overline{Y}_1 + \cdots + \overline{Y}_{i+1}$ belong to the same or adjacent boxes and thus, to the same or adjacent components. Hence, for some i_0 the cell $Y + \overline{Y}_1 + \cdots + \overline{Y}_{i_0}$ belongs to A_i, and the cell $Y + \overline{Y}_1 + \cdots + \overline{Y}_{i_0+1}$ belongs to $\overline{A}$. This yields the contribution $-\frac{1}{2}U(\overline{Y}_{i_0+1}) > 0$ to the sum (5.2). By virtue of the selection of M the cell $Y + \overline{Y}_1 + \cdots + \overline{Y}_{i_0}$ belongs to the box adjacent to that to which Y belongs. Hence, for any box of the outer boundary, we have found a cell Y_1 (this is the cell $Y + \overline{Y}_1 + \cdots + \overline{Y}_{i_0}$), which lies in a box adjacent to the box adjacent to the initial box so that there is a component with the Y_1 in the sum (5.2) which is greater than $-\frac{1}{2}\max_{i=1,\cdots,m} U(\overline{Y}_i)$. Since the set consisting of the initial box, the boxes adjacent to it, and the boxes adjacent to the adjacent box, contains 25 boxes, then a cell Y_1 will be contained in one of each of the 25 boxes of the outer boundary which will yield a contribution not less than $-\frac{1}{2}\max_{i=1,\cdots,m} U(\bar{Y}_i)$ to the sum (5.2), and we have proved (5.1) for

$$d = -\tfrac{1}{50} \max_{i=1,\cdots,m} U(\bar{Y}_i). \tag{5.3}$$

Moreover, let us again assume that the potential is nonperiodic, and nonpositive, but let us demand, instead of finiteness, only compliance with inequality (1.6). We select the side of the box M such that, as before, first $|\bar{Y}_i|$ and $|\bar{Y}_1 + \cdots + \bar{Y}_i|$, $i = 1, \cdots, m$ do not exceed M. The second constraint on M, which replaces the requirement $M > R$, will be mentioned below. The same reasoning as was presented earlier for the finite potential shows that

$$\tfrac{1}{2} \sum_{Y_1 \in F_1, Y_2 \in \bar{F}, \gamma_{Y_1,Y_2} = -1} \gamma_{Y_1,Y_2} U(Y_1 - Y_2) \geq d\, K_i(a); \tag{5.4}$$

however, it is now impossible to state that the members with $\gamma_{Y_1,Y_2} = 1$ are zero, and the sum of these negative members must now also be bounded from below. Let us introduce the following auxiliary concept. We shall call the pair of cells Y_1, Y_2 associated with the box b, if the box b lies between the horizontal on which Y_1 lies and the horizontal on which Y_2 lies, and the vertical on which Y_1 lies passes through the box b, or if the same property is true if Y_2 replaces Y_1 and Y_1 replaces Y_2, or the verticals by the horizontals, and the horizontals by the verticals. Let us show that for any arrangement a and any cells $Y_1 \in \bar{F}$, $Y_2 \in F$ such that $\gamma_{Y_1,Y_2} = 1$, the pair of cells Y_1, Y_2 is associated with one of the boxes of the outer boundary of the considered component of the arrangement A_i, or with one of the boxes adjacent to the boxes of this outer boundary. Indeed, two filled or two empty cells belonging to different components may not belong to the same or to adjacent boxes. Therefore, Y_1 and Y_2 belong to different nonadjacent boxes. Let us draw a path along the boxes from the box in which Y_1 appears to the box in which Y_2 appears so that this path proceeds first along a horizontal and then along a vertical. On this path there is at least one box of the outer boundary, since if the initial and final boxes of the path are not boxes of the outer boundary, then this path will be a path from the upper to the lower boxes, and the required fact was noted in the proof of lemma 4. If this box of the outer boundary is not at the beginning, at the end, or on a turn of the path, it is the desired box. If this is not so, then one of the adjacent boxes of the path is the desired box.

Let us now estimate the sum

$$S = \tfrac{1}{2} \sum U(Y_1 - Y_2) \tag{5.5}$$

over all pairs of cells Y_1 and Y_2 associated with the fixed box b. To do this, let us note that if $\mathfrak{D}_r$ is the set of all cells on the horizontal a distance r from the cell Y, then in conformity with (1.6),

$$\begin{aligned} H_r = \tfrac{1}{2} \sum_{\tilde{Y} \in \mathfrak{D}_r} |U(Y_1 - \tilde{Y})| &\leq \tfrac{1}{2} C \sum_{\tilde{Y} \in \mathfrak{D}_r} |Y - \tilde{Y}|^{-4+\epsilon} \\ &= \tfrac{1}{2} C \sum_{k=-\infty}^{\infty} (k^2 + r^2)^{-(2+1/2\epsilon)}. \end{aligned} \tag{5.6}$$

Replacing this series by an improper integral, it is easy to establish that for some $\overline{C} < \infty$

$$H_r \leq \overline{C}_r^{-(3+\epsilon)}. \tag{5.7}$$

There are $r - M$ pairs of horizontals, spaced a distance r apart, the first of which will be above, and the second below the box with side M. It follows that

$$\begin{aligned} |S| &\leq 4 \sum_{r=M+1}^{\infty} M(r - M)H_r \leq 4\overline{C}M \sum_{r=M+1}^{\omega} (r - M)r^{-(3+\epsilon)} \\ &\leq 4\overline{C}M \sum_{r=M+1}^{\infty} r^{-(2+\epsilon)} \leq \tilde{C}M^{-\epsilon} \end{aligned} \tag{5.8}$$

where $\tilde{C} < \infty$ is a certain constant. Since the total number of boxes of the outer boundary or of the adjacent ones does not exceed $9K_i(a)$, it results from (5.8) that

$$\Big|\tfrac{1}{2} \sum_{Y_1\in\overline{F}, Y_2\in\overline{F}, \gamma_{Y_1,Y_2}=1} \gamma_{Y_1,Y_2}\, U(Y_1 - Y_2)\Big| \leq 9\tilde{C}K_i(a)M^{-\epsilon}. \tag{5.9}$$

Having selected the length of the side of the box M sufficiently large, we may insure that the sum (5.9) does not exceed $\frac{1}{2}\, dK_i(a)$ (let us note that by virtue of the definition (5.3) the value of d is independent of the selection of M), and hence, the statement of lemma 5 results from (5.9) and (5.4) in the case now under consideration.

Let us now assume that condition (1.5) is satisfied and the potential is finite, that is, $U(Y) = 0$ for $|Y| > R$. Then, exactly as in the case of a nonpositive finite potential, by selecting $M > R$ we obtain that $U(Y_1 - Y_2) = 0$ for $\gamma_{Y_1,Y_2} = 1$, and we must estimate only the sum of the terms with $\gamma_{Y_1,Y_2} = -1$. Let us call singular a cell of the arrangement a which belongs to a component A_i and is such that one of the four neighboring cells along the horizontal and vertical belong to the component $\overline{A}$ which is upper for A_i and adjacent to A_i. Let $L_i(a)$ be the number of such singular cells. Since there is a singular cell for each box of the outer boundary in this or an adjacent box, then

$$L_i(a) \geq \tfrac{1}{5}K_i(a). \tag{5.10}$$

Let $Y_0 \in A_i$ be a singular cell and $Y_0 + E$, where E is the unit vector, a cell of the component $\overline{A}$. For any Y with absolute value $|Y| < R$ the cell $Y_0 + Y$ belongs either to a component A_i or $\overline{A}$. This means that either $\gamma_{Y_0,Y_0+Y} = -1$ or $\gamma_{Y_0+E,Y_0+Y} = -1$. Hence, if G_{Y_0} is the set of cells Y_0 and the four cells abutting on the sides of Y_0, then

$$\begin{aligned} &\textstyle\sum' \gamma_{Y_1,Y_2}\, U(Y_1 - Y_2) \\ &\quad \geq \sum_{Y\in\overline{\mathfrak{D}}, Y\in E_2\in\overline{\mathfrak{D}}, \cdots, Y+E_4\in\overline{\mathfrak{D}}} \max\,(U(Y),\, U(Y + E_1),\, \cdots,\, U(Y + E_4)) \end{aligned} \tag{5.11}$$

where the $\sum'$ is taken over pairs of cells Y_1, Y_2 such that $Y_1 \in \overline{F}$, $Y_2 \in F$, $U(Y_1 - Y_2) < 0$ and either Y_1 or Y_2 enters into G_{Y_0}. Since the same cell may belong to G_{Y_0} for not more than the four singular cells of Y_0, then

$$(5.12)\qquad \tfrac{1}{2} \sum_{Y_1\in\bar{F}, Y_2\in F, U(Y_1-Y_2)<0} \gamma_{Y_1,Y_2} U(Y_1 - Y_2)$$
$$\geq \frac{L_i(a)}{\gamma}\Bigg(\sum_{Y\in\bar{\mathfrak{D}}, Y+E_1\in\bar{\mathfrak{D}},\cdots,Y+E_4\in\bar{\mathfrak{D}}} \max\,(U(Y),\, U(Y+E_1),\, \cdots,\, U(Y+E_4))\Bigg).$$

In order to estimate the sum of the members with $U(Y_1 - Y_2) > 0$, let us introduce the following concept. Let us say that the pair of cells Y_1, Y_2 are associated with the cell Y_0 if Y_1 lies on the same horizontal as Y_0, and the vertical on which Y_0 lies passes between the verticals on which Y_1 and Y_2 lie, or coincides with one of these verticals, or, if the same is true when Y_1 is replaced by Y_2 and Y_2 by Y_1 or the verticals by the horizontals and the horizontals by the verticals. Let us note that if $Y_1 \in A_i$, $Y_2 \in \bar{A}$ and $|Y_1 - Y_2| < M$, then the pair Y_1, Y_2 is associated with some singular cell. In fact, the path along the cells from Y_1 to Y_2 which first passes along the horizontal on which Y_1 lies and then along the vertical on which Y_2 lies will contain only cells of the components $\bar{A}$ and A_i, and hence will contain at least one singular cell which will be the desired one. Let us note now that if the vector Y has the components x_1, x_2, then for any cell Y_0 there will be $|x_1| + |x_2| + 1$ pairs of cells Y_1, Y_2 such that $Y_1 - Y_2 = Y_0$ and the pair of cells Y_1, Y_2 will be associated with this cell Y_0 (there are here $|x_2| + 1$ ways of setting Y_1 on the vertical on which Y_0 lies, with one pair in common, arising when Y_1 coincides with Y_0). It follows that for $Y = (x_1, x_2)$

$$(5.13)\qquad \textstyle\sum'' U(Y_1 - Y_2) \leq \displaystyle\sum_{U(Y)>0} (|x_1| + |x_2| + 1)\, U(Y)$$

where the sum $\sum''$ is taken over all pairs of cells Y_1, Y_2 such that $U(Y_1 - Y_2) > 0$ and the pair of cells Y_1, Y_2 is associated with the cell Y_0. Taking into account that $|x_1| + |x_2| + 1 \leq 2(|Y| + 1)$ and that any pair of cells $Y_1 \in \bar{F}$, $Y_2 \in \bar{F}$, for which $U(Y_1 - Y_2) > 0$ is associated with some singular cell, we deduce from (5.13) that

$$(5.14)\qquad \tfrac{1}{2} \sum_{Y_1\in\bar{F}, Y_2\in F, U(Y_1-Y_2)>0} \gamma_{Y_1,Y_2} U(Y_1 - Y_2)$$
$$\geq \tfrac{1}{2} L_i(a) \sum_{U(Y)>0} (|Y| + 1)\, U(Y).$$

(The factor $\frac{1}{2}$ on the right side occurs because $U(Y_1 - Y_2)$ and $U(Y_2 - Y_1)$ entered separately into the right side of (5.13).) From (5.14) and (5.12) and (5.10) it follows that

$$(5.15)\qquad \tfrac{1}{2} \sum_{Y_1\in\bar{F}, Y_2\in F} U(Y_1 - Y_2)$$
$$\geq \frac{K_i(a)}{10}\Bigg[-\sum_{U(Y)>0} (|Y| + 1)\, U(Y) - \tfrac{1}{4} \sum_{Y\in\bar{\mathfrak{D}}, Y+E_1\in\bar{\mathfrak{D}},\cdots,Y+E_4\in\bar{\mathfrak{D}}}$$
$$\max\,(U(Y),\, U(Y+E_1),\, \cdots,\, U(Y+E_4))\Bigg],$$

and since by virtue of the condition (1.5) of the theorem the quantity in the square brackets is positive, then statement (5.1) follows from (5.15).

The extension to the case when (1.5) is true but the finiteness condition is replaced by condition (1.6) is carried out exactly as for the nonpositive potentials. It is only necessary to choose M so large that if the summation in the square brackets will turn out to be greater than $90\tilde{C}M^{-\epsilon}$ (see (5.9)).

6. Conclusion of the proof of the theorem

In this section lemma 6 will be proved. From a comparison of this lemma with lemma 1 the fundamental theorem formulated at the beginning will quickly follow.

LEMMA 6. *If conditions* (1) *and* (2) *of the theorem are satisfied, then for any* $\delta < \frac{1}{2}$ *there exists a* T_δ *such that for* $T < T_\delta$, *some* $\gamma > 0$ *and all* ℓ

$$\Pr_\ell\left\{\frac{N(a)}{\ell^2} < \tfrac{1}{2} - \delta\right\} > \gamma > 0. \tag{6.1}$$

PROOF. Let us first assume that the assumptions of lemma 5 are true. Using lemmas 4 and 5, we find that

$$\begin{aligned}\sum \exp\left\{-\frac{1}{T}W(a)\right\} &\leq \sum_{K_i(a)=K} \exp\left\{-\frac{1}{T}W(T_i(a))\right\}\exp\left\{-\frac{dK}{T}\right\} \\ &\leq \exp\left\{-\frac{dK}{T}\right\}\mathfrak{D}^K \sum_{b:T_i(a)=b,K_i(a)=K} \exp\left\{-\frac{1}{T}W(b)\right\} \\ &\leq \exp\left\{-K\left(\frac{d}{T} - \log\mathfrak{D}\right)\right\}Q(\ell).\end{aligned} \tag{6.2}$$

(See (2.4) for the definition of $Q(\ell)$.) Finally, we deduce from (2.3) that

$$\Pr_\ell\{K_i(a) = K\} \leq \exp\left\{-K\left(+\frac{d}{T} - \log\mathfrak{D}\right)\right\}. \tag{6.3}$$

Let us note now that each component, except the first, lies within its enveloping broken line (see the proof of lemma 2), and since this enveloping broken line goes along the sides of boxes of the outer boundary, the length of the enveloping contour of the components of A_i does not exceed $4MK_i(a)$. But by the isoperimetric inequality, the area within a contour of length L does not exceed $(4\pi)^{-1}L^2$, from which it follows that the total number of cells in the component A_i does not exceed $\hat{C}(K_i(a))^2$, where $\hat{C}$ is a constant independent of a and i. Since any occupied cell belongs to some component of the arrangement which is different from the initial component, then

$$N(a) \leq \hat{C}\sum_{i=1}^{\ell^2} (K_i(a))^2. \tag{6.4}$$

However, it follows from inequality (6.3) that for any $\delta > \frac{1}{2}$, a T_δ may be chosen which is so small that for $T < T_\delta$ the mathematical expectation

$$M(K_i(a))^2 \leq (\tfrac{1}{2} - \delta)\hat{C}^{-1}, \tag{6.5}$$

and from (6.4) it follows that for $T < T_\delta$ the mathematical expectation

$$M\,N(a) \leq (\tfrac{1}{2} - \delta)\ell^2. \tag{6.6}$$

It follows that (6.1) is true.

It still remains to replace the assumptions of lemma 5 by the more general assumptions of the theorem, that is, to replace the assumption of nonperiodicity in the case of a nonpositive potential by the assumption that it is not identically zero. Let the potential be nonpositive, that is let the set $\mathfrak{D}$ be empty. Let us call the integral vectors Y_1 and Y_2 *connected*, if there exists a sequence of integral vectors $\overline{Y}_1, \overline{Y}_2, \cdots, \overline{Y}_m$ such that $U(\overline{Y}_i) < 0$ and $Y_2 = Y_1 + Y_2 + \cdots + \overline{Y}_m$. Evidently, all the integral vectors decompose into nonintersecting classes of mutually connected vectors. Let g be the length of the least vertical vector which is the difference between two vectors of the same class. Then, geometrically it is clear that there will be g^2 classes in all, each of which is a sublattice of the integral lattice. The case $g = 1$ will correspond to the case of a nonperiodic potential. Let $N_j(a)$, $j = 1, \cdots, g^2$ be the number of filled cells belonging to the j-th class. Then

$$N(a) = N_1(a) + N_2(a) + \cdots + N_{g^2}(a). \tag{6.7}$$

The probability distribution, induced by the distribution (2.3), on the arrangements of the cells in the class will again be given by a formula of the same kind, and hence, all the constructions carried out for a nonperiodic potential go over, in a trivial manner, to the case of arrangements in cells of a class, and hence we obtain analogously to (6.6) that for some $T < T_\delta$

$$M\,N_j(a) \leq (\tfrac{1}{2} - \delta)\,\frac{\ell^2}{g^2}. \tag{6.8}$$

The statement of the lemma for the case under consideration follows from (6.7) and (6.8).

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