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ON ONE FORM OF SINGULARITIES IN MODELS OF THE ISING TYPE

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Geometric properties of typical configurations in Ising type models are considered. The corresponding probabilities are studied as functions of the parameters of the Gibbs distribution. It is shown that these probabilities suffer from singularities in the interval $\mu = 0$, $-\beta_{cr} < \beta < \beta_{cr}$.

It is usually considered that models of the Ising type exhibit essential singularities only related to the transition from the totally disordered to the ordered state with nonvanishing magnetization, or are related to the appearance of long-range order. If the Ising model is treated as a model for the classical lattice gas, then the first type of singularity is related to the transition from a one-phase system to a two-phase system.

This point of view is founded on the fact that, considered as functions of the parameters of the system, e.g., temperature and chemical potential, the correlation functions have singularities only at such transition points. There exist however properties of the configurations as a whole, such that the corresponding probabilities exhibit singularities of a different type. These probabilities have no simple expressions in terms of the correlation functions. The purpose of the present paper is to describe these properties and the problems related to them.

1. CONDUCTION PROPERTIES. GEOMETRIC DESCRIPTION

In the lattice gas interpretation of the Ising model an index 1 is attributed to a particle of spin $\frac{1}{2}$ and an index 0 to a particle of spin $-\frac{1}{2}$. Thus to any spin configuration there is associated a configuration of zeros and ones. In the sequel we consider only the two-dimensional case. Let the accessible volume be a square Ω_n of side n, and assume that the particles are situated at the integer-valued sites of a lattice.

We consider the question whether for a given configuration $x = \{x_i\}$, $x_i = 1, 0$ in the volume Ω_n there exists a broken line consisting of horizontal and vertical line segments of unit length, passing only through lattice sites with $x_i = 1$ and joining opposite sides of the square.

If such a broken line exists and joins the vertical (horizontal) sides of Ω_n it is natural to call the configuration x "conducting along the ones in the horizontal (vertical) direction." If such a line does not exist, it is natural to call the appropriate configuration nonconducting along the ones in the corresponding direction. Similarly, one defines conduction along zeros. Conductivity in one direction implies nonconduction in the other. The following list enumerates all logically possible types of configuration from the point of view of conductivity.

1. Conduction along ones in both directions. Nonconduction along zeros in both directions.

1′. Conduction along zeros in both directions. Nonconduction along ones in both directions.

2. Nonconduction along both ones and zeros in both directions.

3. Conduction along ones and zeros in the horizontal direction.

3′. Conduction along ones and zeros in the vertical direction.

4. Conduction along ones in one direction, nonconduction along zeros in both directions, or the same with ones and zeros interchanged.

In order to determine the type to which a given configuration x belongs we surround those sites i where $x_i = 1$ by unit squares. The totality of such squares decomposes into connected components. The boundary of each component is a closed broken line. The boundaries of different components may have only vertices in common.

Thus, to each configuration one associates a definite set of closed contours. Such contours seem to have been used for the first time by Peierls[1] and in the closely related papers of Griffiths[2] and Dobrushin[3]. These contours differ from the contours and graphs used in the well-known cycle of papers by Domb, Sykes and collaborators on virial and other expansions for various lattices and potentials.

Let $\Gamma_1(x), \ldots, \Gamma_k(x)$ denote the boundaries of connected components for the configuration x. Two boundaries $\Gamma_{i_1}(x)$ and $\Gamma_{i_2}(x)$ will be called contiguous if they have a common vertex. The boundaries $\Gamma_{i_1}(x), \ldots, \Gamma_{i_s}(x)$ form a chain if $\Gamma_{i_{r-1}}$ and Γ_{i_r} are contiguous for $r = 1, \ldots, s$. The set of all boundaries can be decomposed into chains.

In terms of the boundaries $\Gamma_1(x), \ldots, \Gamma_k(x)$ the fact that a configuration belongs to one of the enumerated six types is determined in the following way:

1. Among the contours $\Gamma_i(x)$ there is one which intersects all four sides of the square Ω_n.

1′. There does not exist a chain of contours which joins opposite sides of the square.

2. There exists a chain which joins all four sides of the square.

3′. There exists a chain which joins only the vertical sides of the square and which does not intersect the horizontal sides.

3′. There exists a chain which joins only the horizontal sides and does not intersect the vertical sides.

4. It is relatively difficult to describe this type, and we do not give it here, since we will not encounter it below.

It makes sense to investigate conductivity properties also for other lattices. Thus, for a hexagonal lattice the different contours Γ_i constructed in a similar fashion may not have common vertices. Therefore each chain of contours consists in fact of a single contour only. In a certain sense it is more natural to investigate the conductivity of a hexagonal lattice, since here the different components do not intersect at all and are always at a positive distance from one another.

2. THE GIBBS DISTRIBUTION. STUDY OF THE PROBABILITY OF CONDUCTION

Let a Gibbs distribution (grand canonical ensemble) be defined on the configurations x by

$$\rho(x)=\frac{e^{-\beta\Gamma(x)+\mu N(x)}}{\Xi(\beta,\mu/\Omega_n)},$$

where N(x) is the particle number, β and μ are parameters and Ξ is the grand partition function. The parameter β is the reciprocal temperature in units in which the Boltzmann constant is one and μ is the chemical potential multiplied by β. It is convenient to assume that $-\infty < \mu < \infty$, $-\infty < \beta < \infty$. The physical meaning of $\beta < 0$ consists in going from a ferromagnetic Ising model to an antiferromagnetic one. We shall be interested in finding out to which of the six types of configuration a typical configuration belongs for different values of β and μ.

1. Single-phase region for $\mu > 0$. Under these conditions the average density of ones is larger than $1/2$. One can prove rigorously (cf.[4,5]) that for $\beta > \ln 5$ the typical configurations have one large contour which intersects all four sides of the square Ω_n. The length of the remaining contours or chains does not exceed $c(\beta) \ln n$. Thus, in this case the typical configurations belong to the first type. In other words, the probability for conduction along ones in both the horizontal and vertical directions tends to one as $n \to \infty$. It is natural to assume that the configuration type is conserved throughout the whole region under consideration.

2. Single-phase region for $\mu < 0$. Under these conditions the average particle density is smaller than $1/2$. Here for all typical configurations the length of each chain does not exceed $c(\beta\mu) \ln n$, and therefore such a configuration belongs to the first type, i.e., the probabilities of conduction along ones tend to zero, those along zeros tend to one in both directions.

As $\mu \to 0$, $\beta > \beta_{cr}$ the limits which are obtained are different, depending from which side μ approaches the limit. Therefore on the half-line $\mu = 0$, $\beta > \beta_{cr}$ the configuration type depends on additional parameters, e.g., on the boundary conditions.

Thus, outside the half-line $\mu = 0$, $\beta > -\beta_{cr}$ we have in each quadrant of the plane an unchanged configuration type. It will be shown later that in the interval $-\beta_{cr} < \beta < \beta_{cr}$ a new configuration type appears. This means that the whole segment $-\beta_{cr} < \beta < \beta_{cr}$ is critical from the viewpoint of conductivity. The idea that a singularity occurs for density $1/2$ ($\mu = 0$) belongs to I. M. Lifshitz.

3. $-\beta_{cr} < \beta < \beta_{cr}$, $\mu = 0$. The average density of ones is $1/2$ and the configuration is symmetric with respect to an interchange of zeros and ones and vice versa. Here the situation is somewhat different for quadratic and hexagonal lattices.

In the case of a quadratic lattice the typical configurations seem to belong to the second type. A theoretical investigation of this case is fairly complicated even for $\beta = 0$, when the individual coordinates x_i are independent and take on the values 1 and 0 with probabilities $1/2$. We have modeled this case using an electronic computer.

In order to elucidate the conduction properties we have constructed five configurations in a square of 30×30 sites. Random numbers were selected by means of a random number program proposed by Chentsov[6]. All five configurations turned out to belong to the second type. An analysis of these configurations shows that one can traverse a distance along the ones which is by an order smaller than the side of the square.

Further three configurations have been obtained in the rectangle 20×40 (20 is the width). These configurations also turned out to belong to the second type. But here one can traverse along ones a distance of the order of $1/2$ the width.

Apparently if the admissible volume Ω_n is a rectangle for which the ratio between width and length tends to zero, then already for a relatively slow vanishing the typical configurations will turn out to be conducting along ones and zeros in the vertical direction, i.e., will belong to the type 3′. This is true and can be proved theoretically if the width does not exceed a power of $(1/2 - \epsilon)$ of the length for any $\epsilon > 0$.

Thus, for $\beta = 0$ for a square Ω_n the most likely answer is that the typical configurations belong to the third type. As in the other cases, we assume that this type is conserved for the whole interval $-\beta_{cr} < \beta < \beta_{cr}$.

A theoretical investigation of the conduction properties is difficult owing to the absence of an answer to the following question. The geometrical construction of the contours in Sec. 1 can be carried out simply if one has the configuration of particles throughout the whole plane. There appears a new possibility consisting in the appearance of contours of infinite length. If one considers that the probability distribution in the whole plane is the limit of finite-volume Gibbs distributions (cf.[7]), it can happen that there is a positive probability for infinite contours. Logically such a possibility cannot be excluded, although it is little realistic, and seems to be extremely hard to estimate theoretically. We have constructed a computer model for this probability for $\beta = 0$ and various μ.

Each contour Γ which is part of the boundary can be obtained as a trajectory of a random walk of Markov type, but with infinite memory. Let the first step consist in a transition of the broken line l with probability 1 from the point (0, 0) to the point (1, 0). We place at the point $(1/2, 1/2)$ the number 1 and at the point $(1/2, -1/2)$ the number 0.

Assume already constructed a broken line consisting of k segments $l_1, \ldots, l_k$ and such that in the points of the shifted lattice (by $1/2$ in each coordinate) have been placed the numbers 1 and 0. Let the endpoint of the broken line be at the site (i_1, i_2) and the preceding endpoint at the point $(i_1 - 1, i_2)$. Then at the point $(i_1 - 1/2, i_2 + 1/2)$ there will be a 1, and at the site $(i_1 - 1/2, i_2 - 1/2)$ there is a 0. Then at the next step of the random line one will observe the point $z_1 = (i_1 + 1/2, i_2 + 1/2)$. If there already is a 0 at the point z_1, the broken line moves upward with probability 1 and will be at the point $(i_1, i_2 + 1)$. If there is a 1 at z_1 one will observe the point $z_2 = (i_1 + 1/2, i_2 - 1/2)$. If there is a 1 at this point, the broken line will move downward with probability 1, to the point $(i_1, i_2 - 1)$; if there is a 0 the broken line moves horizontally with probability 1 into the point $(i_1 + 1, i_2)$.

If there is no number yet at z_1, one makes a Bernoulli test with probability of success p and failure q. In case of success one puts 1 at z_1 and 0 in case of failure. Now at z_1 there is a number and we repeat the action as explained. If there is no number yet at z_2 we subject it to a Bernoulli test with the same probabilities and continue moving the broken line as explained. Other cases of the position of the last segment are treated analogously.

We are thus led to a random walk. The trajectory of this walk is reversible if the moving point returns to the point (1, 0). The probability of an infinite contour is the probability that the trajectory be irreversible.

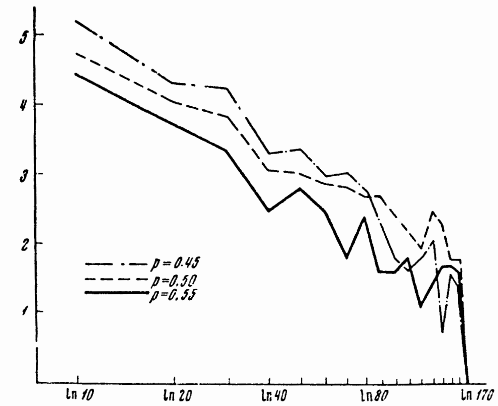
The described random walk was modeled on an electronic computer. The broken line started from the point (0, 0) and the first step was to the point (1, 0). The walk was considered finished either when the broken line returned to the point (1, 0) or when it reached the boundary of a square of side length 30, centered at (0, 0). The count was also terminated if the number of steps exceeded 500. The following results were obtained in this manner:

Thus, for $p = 0.5$ only 4.6% of all the broken lines did not return to the origin. It seems that a substantial majority of the lines which did not return was due to the fact that the computation was done only for a square of side-length 30. As the length of the sides of the square is increased it would seem that these lines would also close. From the results of the computation at $p = 0.5$ it seems most likely to hypothesize that the probability of an infinite contour vanishes.

The results of a computation for $p = 0.45$ show that the typical picture of the contours is the following. There are exterior contours which are not surrounded by any other contours. Exterior to these contours there are zeros, interior, there are ones. Inside these extreme contours there are contours which have ones to the outside and zeros to the inside. The results of the computation referred probably to these latter types, and this explains why they all closed.

For $p = 0.55$ the preceding picture changes in the sense that the zeros are replaced by one and conversely.

Total number of broken lines	Number of closed broken lines	Probability of ones	Number of broken lines going to the boundary of the square	Number of broken lines which did not close after 500 steps and stayed inside the square
0.5	480	458	21	1
0.45	480	480	0	0
0.55	480	306	154	20



Now the counting refers to the external contours and to the internal contours inside them which have ones on the outside. It is natural to expect that the 174 lines for which the computation was interrupted correspond to external contours. It follows that the fraction of external contours is not smaller than 35%; this shows that the disappearance of external contours for $p = 0.5$ goes on pretty sharply.

If one considers that for $p = 1/2$ the probability of infinite contours vanishes, one obtains the formula

$$\pi = \sum_{1}^{\infty} n \sum_{\text{length of } \Gamma = n} p(\Gamma) \leqslant 2,$$

where π is the average number of segments in the lattice which belong to the boundary of the configuration (the number of segments in the square Ω_n equals $2n^2$). On the other hand it is easy to show that

$$\sum n^2 \sum_{\text{length of } \Gamma = n} p(\Gamma) = \infty.$$

This implies that the probability for a contour of length n decreases according to a power law, with exponent between 1 and 2. We have constructed a histogram of the distribution on a sample of 480 contours. Its form in a logarithmic scale is given in the figure. It shows that the most probable value of the power is one.

For $\mu \neq 0$ the appropriate distribution decays exponentially. Apparently the exponent has a singularity for $\mu = 0$ along the whole segment $|\beta| < \beta_{cr}$, but the character of this singularity is unknown.

For $\beta < -\beta_{cr}$ there is a curve separating the antiferromagnetic phase from the disordered phase. From the point of view of conductivity the configurations with antiferromagnetism belong to the second type. Thus, inside this curve the typical configurations belong to the second type. It is likely that the separation curve also serves as a curve of singularities.

The expounded facts referred to a square lattice. For a hexagonal lattice the situation for the segment $|\beta| < \beta_{cr}$, $\mu = 0$ seems to be changed. No chains of contours are possible in this case and therefore here configurations of the second type have a substantially lower entropy, and therefore their probability tends to zero.

In this case the existence of a limiting contour which connects the opposite sides of a square Ω_n implies that the conduction along ones in any direction leads to conduction along zeros in the same direction.

Owing to isotropy, the probabilities of conduction in the horizontal and vertical directions are asymptotically equal to $1/2$. However, if one fixes a typical configuration in the whole plane and investigates the conduction properties inside the square Ω_n, this property will vary quite irregularly with the variation of n. For about half of the values of n there will be horizontal conduction, and for about half, vertical conductivity.

The contents of this paper are also related to the problems referring to the so-called "soaking" problems (cf. in particular the papers of M. Fisher[8], Hammersley[9] and Elliott et al.[10]).

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