Broken Symmetry and Domain Structure in Ising-like Systems

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In Ising-like systems, there is a temperature T^*, strictly between zero and the usual critical temperature, above which any region of arbitrary size is completely contained within a domain which prefers energetically to be flipped.

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Consider a d-dimensional lattice spin system with a discrete symmetry group, such as the standard d-dimensional Ising ferromagnet. Suppose that at temperature T any region, at any location and of arbitrary size, is contained within some larger domain such that a fixed rotation of all spins within this domain relative to those outside would lower the energy. It has been argued that such a situation is inconsistent with spontaneously broken symmetry.[1] This conclusion appears self-evident since such domains would seemingly decouple the bulk from boundary conditions at infinity.

Nevertheless, this conclusion is wrong for nearest-neighbor Ising models (and Potts models with second-order phase transitions) in any dimension. In this Letter, we confine ourselves to providing a proof for the simplest case, that of the two-dimensional Ising ferromagnet. A future paper will cover higher dimensions and Potts models. We will also show here that the *converse* conclusion is correct for Ising ferromagnets in any dimension; i.e., the absence of such large-scale domains at temperature T implies the existence of broken symmetry.

Our results can alternatively be viewed by considering the probability of finding, in a typical configuration of the broken-symmetric phase, a surface surrounding a large cube of volume L^d such that a rigid flip of the enclosed spins will lower the energy. At sufficiently low temperature it is clear, and easy to show using a Peierls-type argument, that the probability of finding such a domain is bounded from above by $\exp[-c(T)L^{d-1}]$, where $c(T)>0$. In the paramagnetic phase it seems obvious that this probability should equal 1 independently of L, i.e., that $c(T)=0$, $T>T_c$ (we, in fact, prove this assertion later). It then seems natural to suppose that $c(T)\rightarrow 0^+$ only when $T\rightarrow T_c^-$. We find, however, that $c(T)=0$ above a new temperature T^* strictly between 0 and T_c.[2]

To state our results precisely, we introduce some definitions. By a domain, we mean a finite connected subset V of Z^d with no holes; i.e., every pair of sites in V can be connected by a nearest-neighbor path in V, and every pair of sites not in V can be connected by a nearest-neighbor path not in V. Given an Ising spin configuration $\sigma=(\sigma_x: x\in Z^d)$ and a domain V, we denote by σ^V the spin configuration which is the negative of σ in V and the same as σ outside of V. Given a Hamiltonian $\mathcal{H}$, we say that a domain V has positive energy if $\mathcal{H}(\sigma^V)-\mathcal{H}(\sigma)<0$ [and non-negative energy if $\mathcal{H}(\sigma^V)-\mathcal{H}(\sigma)\le 0$]. For the standard nearest-neighbor Ising ferromagnet with

$$\mathcal{H}=-\sum_{\langle x,y\rangle}\sigma_x\sigma_y\,, \tag{1}$$

this is equivalent to the surface of V (denoted $\partial V\equiv\{\langle x,y\rangle$ with x in V and y not in $V\}$) having more unsatisfied bonds than satisfied ones: $N_V^u>N_V^s$, where N_V^u is the number of $\langle x,y\rangle$ in ∂V with $\sigma_x\neq\sigma_y$ and N_V^s is the number of $\langle x,y\rangle$ in ∂V with $\sigma_x=\sigma_y$. That is, it is energetically advantageous for the system to "flip" a positive-energy domain.

As stated earlier, it is not difficult to prove that at very low temperatures, typical spin configurations have few positive-energy domains, while at high temperature they have many. Here "many" means that for each length scale L, there exists a positive-energy domain Λ_L containing the box $B_L\equiv[-L,L]^d$; "typical" refers to a set of spin configurations having probability 1 in an appropriate infinite-volume Gibbs distribution.

Of greater interest is the relation at intermediate temperatures between the sparseness of positive-energy domains and the nonvanishing of the spontaneous magnetization $M(T)$.

Theorem A.—In the standard 2D Ising ferromagnet, there is a T^* strictly less than the critical temperature T_c such that, for all T satisfying $T^*<T<T_c$, typical spin configurations in the positively magnetized, pure phase at temperature T have many positive-energy domains.

Given this result, one might suppose that the entropy of the surfaces surrounding positive-energy domains is vanishingly small, so that their free energy is negligible. Surprisingly, this is not the case: Arguments given below show that usually the surface containing an arbitrary $L\times L$ square is mostly within a distance ~ 1 from the square, and the number of such surfaces contained between the $L\times L$ square and a surrounding $2L\times 2L$ square grows exponentially with L. Furthermore, one can estimate the maximum distance of the domain surface from the square: There is a positive fraction of the L's for which Λ_L can be chosen within $B_{L'}$ with $L'-L = O(\ln L)$ as $L \rightarrow \infty$. For these L's, the total magnetization in Λ_L (before flipping the spins) is essentially $M[(2L)^2]+o(L^2)$ so that the flipped configuration has a *negative* magnetization per site in Λ_L, but still a lower energy.

Theorem A shows that the presence of many positive-energy domains does *not* guarantee the absence of symmetry breaking. On the other hand, the next theorem shows, at least for Ising ferromagnets, that the *absence* of large-scale, positive-energy domains *does* imply the presence of symmetry breaking; a natural extension of our arguments can be applied to Potts ferromagnets to obtain an analogous result.

Theorem B.— In the standard d-dimensional Ising ferromagnet, if $M(T)=0$, then typical spin configurations (in the unique phase) at temperature T have many nonnegative energy domains.

Theorem A is based on an analysis of parallel spin clusters which relies on the result of Coniglio *et al.*[3] that, in two dimensions, infinite plus and minus clusters cannot coexist.[4] Thus, for $T < T_c$, the plus phase contains an infinite plus cluster but no infinite minus cluster, while for $T \geq T_c$ there exist no infinite clusters of either sign. The physical idea behind the proof is as follows. Consider an $L \times L$ square in the plus phase. For L large enough, the square will intersect the infinite plus cluster with probability close to 1. To obtain a positive-energy domain, construct its surface as a closed loop which contains the intersection of the boundary of the square with the infinite cluster, and continues outside the square only along boundaries between plus and minus clusters (see Fig. 1). The distance one needs to go out to obtain such a loop is determined by the size of the finite clusters overlapping the boundary of the original square. Such a closed loop is guaranteed to exist for $T < T_c$ because there are no infinite minus clusters. The fact that the finite clusters overlapping an $L \times L$ square are all of order $\ln L$ or smaller justifies the remark following Theorem A. The only negative contribution to the surface energy is bounded from above by the intersection of the square boundary with the infinite cluster, but this becomes a negligible fraction of the total boundary as $T \rightarrow T_c^-$ because the infinite cluster density vanishes at T_c (in fact, having this fraction of the perimeter less than $\frac{1}{2}$ is sufficient). The technical proof now follows.

From here on we will work in the $T < T_c$ plus phase. Let us denote by ∂_L the *sites* in B_L which have a nearest

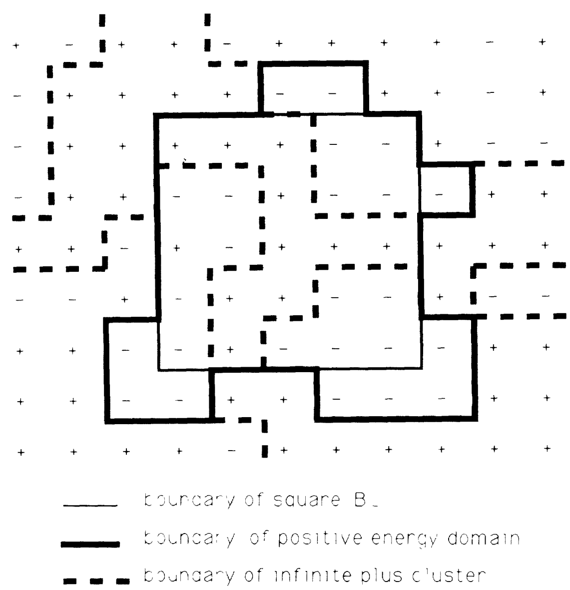

FIG. 1. A sketch of the construction used in Theorem A. The boundary $\partial\tilde{\Lambda}_L$ encloses the positive-energy domain which contains the $L \times L$ square B_L.

neighbor outside B_L and decompose it into three parts:

$$\partial^i_L = \{x \in \partial_L:\ \text{the cluster of } x \text{ is infinite}\},$$

$$\partial^{\pm}_L = \{x \in \partial_L:\ \sigma_x = \pm 1 \text{ and the cluster of } x \text{ is finite}\}.$$

We have therefore separated sites on the boundary into those belonging to the infinite plus cluster and those belonging to finite plus or minus clusters (which may be as small as a single spin). For x in $\partial^{\pm}_L$, we define C_x as the (plus or minus) cluster to which x belongs. Each such C_x is finite.

Our candidate for the positive-energy domain Λ_L is $\tilde{\Lambda}_L$, the union of B_L with all of these C_x's (and all resulting holes); see Fig. 1. Each $\langle x,y\rangle$ in $\partial\tilde{\Lambda}_L$ either has x from one of the C_x's, in which case $\sigma_x \neq \sigma_y$, or else has x from ∂^i_L. Since the length $|\partial_L|$ of ∂_L is no larger than that of $\partial\tilde{\Lambda}_L$, we see that [up to terms of $O(1)$ coming from corners]

$$N^u_{\tilde{\Lambda}_L} \geq |\partial_L| - |\partial^i_L|,\quad N^s_{\tilde{\Lambda}_L} \leq |\partial^i_L|. \tag{2}$$

Thus Λ_L can be taken as $\tilde{\Lambda}_L$ providing $|\partial^i_L| < \frac{1}{2}|\partial_L|$. We show below that this inequality will be satisfied for a positive fraction of L's; when not satisfied for a *given* L, choose Λ_L as the smallest $\tilde{\Lambda}_l$ with $l > L$ for which $|\partial^i_l| \leq \frac{1}{2}|\partial_L|$.

Now, by ergodicity, we can relate $|\partial^i_L|/|\partial_L|$ to the spin percolation density $R(T)$. Consider a big square of size L' as the union of boundaries of squares of smaller size. Then as $L' \rightarrow \infty$

$$(2L'+1)^{-2}\sum_{L=0}^{L'}|\partial^i_L| = \text{fraction of sites of } B_{L'} \text{ in the infinite cluster}$$
$$\rightarrow R(T) = \Pr(\text{the origin belongs to the infinite cluster}). \tag{3}$$

This implies that $|\partial^i_L| < \frac{1}{2}|\partial_L|$ will be satisfied for (at least) a positive fraction of L's if $R(T) < \frac{1}{2}$. To complete the proof, we need only show that $R(T) \to 0$ as $T \to T_c^-$. This follows from the fact that there is no percolation at T_c, so that $R(T_c)=0$, and that by the inequalities of Fortuin, Kesteleyn, and Ginibre[5] $R(T)$ is a decreasing limit of finite-volume approximations.[6]

To show that $\tilde{\Lambda}_L$ is contained in B_l with $l-L=O(\ln L)$, justifying the remark following Theorem A, we need to show that the maximum diameter of the C_x's is $O(\ln L)$. To show this, it suffices by standard probabilistic arguments to have

$$\sum_{L \geq L'} \sum_{x \in \partial_L} \Pr(\text{diam of } C_x \geq c_1 \ln L) \to 0 \text{ as } L' \to \infty\,, \quad (4)$$

for some $c_1(T) < \infty$ (here we define C_x to be empty if $x \in \partial_L^i$). This will be the case if

$$\Pr(\text{diam of } C_x \geq k) = O(e^{-c_2 k})\,,$$

since at fixed T we can always choose c_1 such that $c_1 c_2 > 2$. To obtain this latter estimate we note that for x in ∂_L^+ the minus spins in the clusters adjoining C_x are $*$-connected (i.e., by paths which can go to diagonal neighbors); thus it suffices to show that

$$\Pr(\text{origin belongs to or is enclosed by a minus } *\text{-cluster of diam} \geq k) = O(e^{-c_2 k})\,.$$

This in turn easily follows from the fact that the two-point connectivity function for minus $*$-clusters has a finite correlation length for $T < T_c$.[7]

Theorem A indicates the presence of a new temperature T^* which signals a geometric transition in the prevalence of positive-energy surfaces. Although there is no singularity in the free energy associated with this transition, it may turn out to have other interesting manifestations.

Theorem B is based on an analysis of clusters in the related Fortuin-Kasteleyn (FK) random-cluster model.[8-10] When $M=0$ in the ferromagnet, all FK clusters are finite. Given an FK configuration, corresponding spin configurations are generated by tossing independent fair coins, one for each FK cluster, and assigning all spins in the cluster the value $+1$ for heads and -1 for tails. Now suppose that, prior to tossing coins but after choosing an FK configuration, we generate a sequence of candidates for Λ_L as follows. $\tilde{\Lambda}_{L,1}$ is the union of all FK clusters of the sites in B_L (and all resulting holes). $\tilde{\Lambda}_{L,k+1}$ adds to $\tilde{\Lambda}_{L,k}$ all adjoining FK clusters (and all resulting holes). Suppose we toss coins first for clusters in $\tilde{\Lambda}_{L,1}$, then in $\tilde{\Lambda}_{L,2}-\tilde{\Lambda}_{L,1}$, etc. By a simple symmetry argument, prior to tossing coins for $\tilde{\Lambda}_{L,k+1}-\tilde{\Lambda}_{L,k}$, every outcome of the coin tosses can be paired with that in which the spins in $\tilde{\Lambda}_{L,k+1}-\tilde{\Lambda}_{L,k}$ come out exactly the opposite. If one outcome gives a non-positive energy for $\tilde{\Lambda}_{L,k}$ then the other one gives a non-negative energy. Thus, there is always a conditional probability $\geq \frac{1}{2}$ that $\tilde{\Lambda}_{L,k}$ will have non-negative energy. The probability that $\tilde{\Lambda}_{L,k}$ will have non-negative energy for some $k \leq k'$ is evidently $\geq 1-2^{-k'}$ and thus, with probability 1, eventually *some* $\tilde{\Lambda}_{L,k}$ will have non-negative energy.

A weaker version of Theorem B can be extended to *any* Ising model with arbitrary couplings, including spin glasses. There always exists a temperature $T' \geq T_c$ such that, for all $T > T'$, typical spin configurations in the (unique) phase at that T have many non-negative-energy domains. This temperature corresponds to the percolation transition of an associated FK model.[11]

We have therefore shown that absence of FK percolation implies, for a general Ising model in d dimensions, that a box on any length scale L is contained within a domain whose inversion is either energetically favorable or at least neutral. Since this temperature region is always within the paramagnetic phase, our result is expected. Surprisingly, however, the converse fails. For a two-dimensional system with discrete spin symmetry, we have shown that a temperature region exists *within the broken-symmetry phase* such that a region of *any* size is completely contained within a domain which can be flipped such that the energy is lowered. Moreover, the magnetization within the flipped domain will generally have a sign inconsistent with the majority phase, as determined by the boundary conditions.

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[1]See, for example, A. Bovier and J. Fröhlich, J. Stat. Phys. **44**, 347 (1986), Sec. 5.

[2]It is of course true that the relevant quantity for studying the thermodynamic phase transition is free energy rather than energy. By focusing, however, on energies of typical configurations one might hope to arrive at alternative, useful measures of broken symmetry. Such considerations lead in our situation to the uncovering of the temperature T^*.

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[4]Although the arguments presented here are valid only in two dimensions, it appears that a similar conclusion can be reached in higher dimensions using a construction which takes *advantage* of the coexistence of infinite plus and minus clusters just below T_c. This construction was arrived at in discussions with J. Bricmont and A. Sokal and will appear in a future paper.

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