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Topological conditions for discrete symmetry breaking and phase transitions

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Abstract

In the framework of a recently proposed topological approach to phase transitions, some sufficient conditions ensuring the presence of the spontaneous breaking of a \mathbb{Z}_2 symmetry and of a symmetry-breaking phase transition are introduced and discussed. A very simple model, which we refer to as the hypercubic model, is introduced and solved. The main purpose of this model is that of illustrating the content of the sufficient conditions, but it is interesting also in itself due to its simplicity. Then some mean-field models already known in the literature are discussed in the light of the sufficient conditions introduced here.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Phase transitions are very common in nature. They are sudden changes of the macroscopic behaviour of a natural system composed by many interacting parts occurring while an external parameter is smoothly varied. Phase transitions are an example of *emergent* behaviour, i.e., of collective properties having no direct counterpart in the dynamics or structure of individual atoms [1]. The successful description of phase transitions starting from the properties of the microscopic interactions² between the components of the system is one of the major

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² Here the term 'microscopic' must be understood in a wide sense, i.e., it refers to the interactions between the degrees of freedom entering the Hamiltonian of the system. It might denote the truly microscopic interactions between fundamental particles, atoms, or molecules, or it may refer only to the interactions between relevant degrees of freedom, as in spin systems, as well as to any interaction between the individual components of the system, which may not be microscopic at all: in the studies of the phase transitions occurring in systems interacting via 1/r potentials, the 'microscopic' interactions could be gravitational forces between stars or even galaxies.

achievements of equilibrium statistical mechanics. From a statistical-mechanical point of view, in the canonical ensemble, describing a system at constant temperature T, a phase transition occurs at special values of the temperature called transition points, where thermodynamic quantities such as pressure, magnetization, or heat capacity, are non-analytic functions of T; these points are the boundaries between different phases of the system. Starting from the celebrated solution of the two-dimensional Ising model by Onsager [2], these singularities have been indeed found in many models, and later developments like the renormalization group theory [3] have considerably deepened our knowledge of the properties of the transition points, at least in the case of continuous transitions, or critical phenomena.

Yet, the situation is not completely satisfactory. First, in the canonical ensemble these singularities occur only in the rather artificial case of infinite systems: following an early suggestion by Kramers [4], Lee and Yang [5] showed that the thermodynamic limit $N \to \infty$ (N is the number of degrees of freedom, and the limit is taken at fixed density) must be invoked to explain the existence of true singularities in the canonical partition function Z(T) and then in the thermodynamic functions defined as derivatives of Z(T). Since in the last decades many examples of transitional phenomena in systems far from the thermodynamic limit have been found (e.g., in nuclei, atomic clusters, biopolymers), a description of phase transitions valid also for finite systems would be desirable. Second, while necessary conditions for the presence of a phase transition can be found (one example is the above-mentioned need of the thermodynamic limit in the canonical ensemble), nothing general is known about sufficient conditions: no general procedure is at hand to tell if a system where a phase transition is not ruled out from the beginning does have or not such a transition without computing Z: only for some particular systems or class of systems one can devise $ad\ hoc$ procedures. This might indicate that our deep understanding of this phenomenon is still incomplete.

These considerations motivate a study of the deep nature of phase transitions which may also be based on alternative approaches. One of such approaches, proposed in [6] and developed later [7], is based on simple concepts and tools drawn from differential geometry and topology. The main issue of this new approach is a topological hypothesis, whose content is that at their deepest level phase transitions are due to a topology change of suitable submanifolds of configuration space, those where the system 'lives' as the number of its degrees of freedom becomes very large. This idea has been discussed and tested in many recent papers [8–19]. Moreover, the topological hypothesis has been given a rigorous background by a theorem [20] which states that, at least for systems with short-ranged interactions and confining potentials, topology changes in configuration space submanifolds are a necessary condition for a phase transition. However, the converse is not true (there are topology changes which are *not* connected with a phase transition [12]), and no *sufficient* topological conditions have been obtained yet. The problem of finding the *sufficient* conditions for a phase transition remains one of the fundamental open problems in this field: an answer to this problem would also make the topological approach an ideal candidate to define phase transitions in finite systems, for topology changes in the relevant submanifolds of configuration space do occur in finite systems, so that a criterion to discriminate the 'good' ones would make them a natural extension of the concept of a phase transition to finite N case.

The present paper aims at contributing to the search for topological sufficient conditions by considering, instead of the general problem of a generic phase transition, the more particular—but still very general and important from a physical point of view—case of the spontaneous breaking of a discrete symmetry. Although a phase transition is a far more general phenomenon, which is linked in general with the breaking of ergodicity [3, 21] and may or may not be accompanied by the spontaneous breaking of a symmetry, many interesting phase transitions do occur in nature via the breaking of a symmetry. One of the most familiar

cases is ferromagnetism: in the ordered phase the (continuous) rotational O(3) symmetry of Heisenberg magnets is spontaneously broken. As to discrete symmetries, the paradigmatic example is the Ising model on a lattice, or, if one wants to consider continuous variables, the lattice φ^4 model, where if $d \ge 2$ a ferromagnetic transition exists and is accompanied by the breaking of the global \mathbb{Z}_2 symmetry of the Hamiltonian, i.e., the symmetry under the simultaneous reversal of all the variables (the two-valued spins s_i for the Ising model or the continuous real variables φ_i for the lattice φ^4 model).

In the following we will consider only the case of a \mathbb{Z}_2 symmetry, even if we believe that it should be possible to extend our results to general discrete symmetries. We shall also restrict ourselves to systems described by continuous variables, because the topological approach can be defined only for these systems, even if in some cases we may refer to Ising-like discrete spin systems for illustrative purposes. As we will show in section 3, under fairly general assumptions it is possible to state a sufficient condition for the presence of a \mathbb{Z}_2 -symmetry breaking phase transition essentially in terms of the topology of the equipotential hypersurfaces in configuration space, provided some additional conditions on the behaviour with N are satisfied. Before stating and discussing these results, in section 2 we will discuss at a general level the problem of the breaking of a \mathbb{Z}_2 symmetry and the basis of the topological approach. Then, after having stated the above-mentioned result, in section 4 we will illustrate it introducing a simple abstract model, and in section 5 we will discuss them in the light of some physical models already studied in the literature. We will end with some concluding remarks in section 6.

2. General picture

2.1. Phase transitions with \mathbb{Z}_2 -symmetry breaking

At a qualitative level, the physical mechanism underlying the spontaneous breaking of a \mathbb{Z}_2 symmetry is quite well understood [22]. To begin with, let us consider a simple example with a single degree of freedom: a particle of unit mass in a double-well potential V(q), such that V(q) = V(-q), at a fixed temperature T. The dynamics of the particle will be described by a Langevin equation

$$\ddot{q} = -\gamma \dot{q} - \frac{\mathrm{d}V}{\mathrm{d}q} + \eta(t),\tag{1}$$

where $\eta(t)$ is a δ -correlated white noise whose amplitude is related to the friction coefficient γ and to the temperature by the fluctuation-dissipation theorem,

$$\langle \eta(t)\eta(t+\tau)\rangle = 2\gamma T\delta(\tau).$$
 (2)

The 'magnetization', i.e., the order parameter of the system, whose nonzero value signals the breaking of the \mathbb{Z}_2 symmetry, is the time average of the position q. As long as the temperature is low, the dynamics of the particle is essentially an activated process, with two widely separated time scales: one small scale in which the particle oscillates in one of the two wells, and a large time scale τ in which one observes jumps from one well to the other. On time scales $t \ll \tau$, the symmetry appears to be broken, because the particle is confined in one of the two wells and the finite-time order parameter is nonzero:

$$\frac{1}{t} \int_0^t q(t') \, \mathrm{d}t' \neq 0 \qquad t \ll \tau. \tag{3}$$

According to Kramers' theory [23],

$$\tau \propto \exp\left(\frac{\Delta E}{T}\right),$$
 (4)

where we have set $k_B = 1$ as we shall always do from now on, ΔE is the height of the energy barrier the particle has to overcome in order to jump from the minimum of one well to the other, and is a finite quantity if V is the potential energy of a single particle, so that, even if the time scale τ increases exponentially while decreasing the temperature, the order parameter $\langle q \rangle$ vanishes for any finite temperature:

$$\langle q \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t q(t') \, \mathrm{d}t' = 0 \qquad \forall T > 0, \tag{5}$$

and symmetry breaking is possible only at T=0. Note that increasing ΔE does not change the situation, unless one takes the limit $\Delta E \to \infty$ where the symmetry is broken for any value of T. In any case, no phase transition between a symmetric and a broken-symmetry phase is allowed in this single-particle system.

Nonetheless, we are interested in many-particle systems: it is just the number of degrees of freedom, N, which plays a fundamental role to make a symmetry breaking possible [22]. The potential energy $V(q_1,\ldots,q_N)$ is now a function of N variables, still \mathbb{Z}_2 -symmetric, i.e., $V(q_1,\ldots,q_N)=V(-q_1,\ldots,-q_N)$. The potential energy necessarily has two equivalent absolute minima related by the symmetry, but multidimensionality of configuration space means that there could be many possible routes to go from one minimum to the other. If now we denote by ΔE the *minimum* barrier to jump in order to connect the two minima, for low enough T equation (4) still holds³. This means that, if ΔE grows with N, in the thermodynamic limit the equilibration time scale τ becomes infinite and the system is trapped in one of the two wells even for infinite times: the order parameter $\frac{1}{N} \langle \sum_{i=1}^N q_i \rangle$ is now finite,

$$\frac{1}{N} \left\langle \sum_{i=1}^{N} q_i \right\rangle = \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{Nt} \int_0^t \sum_{i=1}^{N} q_i(t') \, \mathrm{d}t' \neq 0 \qquad \forall T < T_c, \tag{6}$$

and the symmetry is broken for finite temperatures below a critical temperature T_c . Note that in equation (6) the two limits *do not* commute, i.e., we must first let the system go to the thermodynamic limit and then take the infinite-time averages. Doing the other way round we would not get any transition, and no symmetry breaking would be present [22].

The reason why this happens only for $T < T_c$ and not for any T is due on one hand to the fact that the separation of time scales, and thus the activated process picture, holds only for sufficiently low temperatures, and on the other hand to that the above discussion is oversimplified: we have neglected the role of entropy, and the high dimensionality of the configuration space ensures that for sufficiently high T's the entropy will always disorder the system. The above argument could be made more stringent using free energy barriers instead of energy barriers. However, our purpose was only to show, using an intuitive dynamical argument, how in a many-particle system symmetry breaking can occur in the thermodynamic limit, not to prove that it does occur. We have thus seen that one of the basic ingredients for the possibility of symmetry breaking is, besides the thermodynamic limit, that the height of the minimum barrier to overcome must grow with N: here is where, among other factors, the dimensionality of the system comes in. To make a familiar example, in one-dimensional Ising systems ΔE is constant as N grows, because after having flipped one spin all the others can be flipped without any extra energy cost, while is proportional to \sqrt{N} in a two-dimensional system, because to flip a whole region of spins the energy is paid at the perimeter of the region, whose length scales as L^{d-1} for a d-dimensional lattice of length L. We recognize here

³ Equation (4) can indeed be generalized to a multidimensional situation [24]. The multiplicative factors neglected in equation (4), which in the single-particle case are essentially dimensional constants but now account for the entropic contribution, i.e., for the width of the wells and for the width of the saddle to cross, are more complicated and important but this does not affect our reasoning which remains at a qualitative level.

the Landau–Peierls argument [25] to prove the existence of a finite-temperature symmetry breaking in a two-dimensional Ising system, and indeed the physical content of this argument is the same of the 'dynamical' argument above, as to the energy part. The Landau–Peierls argument is much more powerful because the entropic contribution, and then T_c , can be estimated too, provided we can efficiently count the relevant configurations, which however limits its applicability to Ising-like systems. The dynamical argument is valid for general systems with continuous variables, but remains at a qualitative level and does not provide a clear sufficient condition for the presence of a phase transition. As we shall see in the following, it is possible to translate it into the topological language, which does allow to state such a sufficient condition. But before doing that let us review the basis of the topological approach.

2.2. Basis of the topological approach

As already mentioned in the introduction, where also relevant references to original papers were given, the topological approach to phase transitions is based on the 'topological hypothesis' that phase transitions are due to suitable topology changes in some submanifolds of configuration space defined by the potential energy function. Here we want to recall which is the basis of this approach.

Let us consider a Hamiltonian system with N degrees of freedom and standard kinetic energy, described by the Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + V(q_1, \dots, q_N), \tag{7}$$

where V(q) (from now on $q = \{q\}_{i=1}^N$) is the potential energy and the q_i 's and the p_i 's (i = 1, ..., N) are, respectively, the canonical conjugate coordinates and momenta, and are continuous variables; $q \in M$, where M is the N-dimensional configuration space manifold, and V is bounded below on M. The configurational partition function of such a system can be written as (we omit the $(h^N N!)^{-1}$ normalization factor because it is irrelevant for our discussion)

$$Z_N(\beta) = \int_0^\infty d(Nv) e^{-\beta Nv} \omega_N(v), \tag{8}$$

where $\beta = T^{-1}$ and $\omega_N(v)$ is the density of states at (potential) energy per degree of freedom v, i.e., the Liouville measure of the isopotential hypersurface Σ_v ,

$$\omega_N(v) = \mu(\Sigma_v) = \int_{\Sigma_v} \frac{\mathrm{d}\Sigma}{\|\nabla V\|},\tag{9}$$

where Σ_v is defined as the Nv-level set of the potential energy V(q),

$$\Sigma_v = \{ q \in M | V(q_1, \dots, q_N) = Nv \},$$
 (10)

and $d\Sigma$ is the volume element on Σ_v . We write ω_N as

$$\omega_N(v) = (a_N(v))^N, \tag{11}$$

where $a_N(v) = \exp[s_N(v)]$ and $s_N(v)$ is the configurational entropy per degree of freedom. Now we can write (without loss of generality, we assume that the absolute minimum of V is zero)

$$Z_N(\beta) = N \int_0^\infty dv \, e^{N(\log a_N(v) - \beta v)},\tag{12}$$

and then, as N gets very large, we can evaluate the integral over v in (8) by replacing it with the largest value of the integrand:

$$Z_N(\beta) = \operatorname{const} e^{N[\sup_v (\log a_N(v) - \beta v)]}, \tag{13}$$

where up to now we have only assumed extensivity, i.e.,

$$a(v) = \lim_{N \to \infty} a_N(v) = [\mu(\Sigma_v)]^{1/N}$$
(14)

exists and is finite, which, due to the physical meaning of the density of states, amounts to requiring that the specific configurational entropy is well defined in the thermodynamic limit⁴; then we can write

$$Z_N(\beta) \underset{N \to \infty}{\longrightarrow} N e^{-N\beta \overline{v}(\beta)} \mu(\Sigma_{\overline{v}(\beta)}) = N e^{-N\beta \overline{v}(\beta)} \int_{\Sigma_{\overline{v}(\beta)}} \frac{d\Sigma}{\|\nabla V\|}, \tag{15}$$

showing that the only relevant contribution to the partition function comes from a single isopotential hypersurface $\Sigma_{\overline{v}(\beta)}$, where $\overline{v}(\beta)$ is the value of v which realizes the supremum in equation (13); if we assume that the function $\beta v - \log a(v)$ has a single minimum which does not coincide with the extrema of the interval of definition, $\overline{v}(\beta)$ is the solution of the saddle-point equation

$$\frac{\mathrm{d}}{\mathrm{d}\beta}[\beta v - \log a(v)] = 0,\tag{16}$$

and coincides with the expectation value of V/N,

$$\overline{v}(\beta) = \frac{1}{N} \langle V \rangle = -\frac{1}{N} \frac{\partial \log Z_N(\beta)}{\partial \beta}.$$
 (17)

This amounts to saying that as $N \to \infty$ the support of the equilibrium measure reduces to the equipotential hypersurface $\Sigma_{\overline{v}(\beta)}$. In other terms, when computing the canonical ensemble average of a function A(q), we can write as N gets very large

$$\langle A \rangle(\beta) \underset{N \to \infty}{\longrightarrow} = \frac{1}{\tilde{Z}(\beta)} \int_{\Sigma_{\tilde{\Pi}(\beta)}} \frac{A|_{\Sigma} d\Sigma}{\|\nabla V\|}, \tag{18}$$

where $A|_{\Sigma}$ is the restriction of the function A(q) to $\Sigma_{\overline{v}(\beta)}$ and

$$\tilde{Z}(\beta) = \int_{\Sigma_{\overline{u}(\beta)}} \frac{\mathrm{d}\Sigma}{\|\nabla V\|}.$$
(19)

A major topology change in a family of manifolds, depending on a continuous parameter v, occurring at some v_c may induce singularities in the v-dependence of their volume, whence the basic idea of the topological hypothesis: the deep origin of a phase transition might be concealed in the way the configuration space is foliated in level sets of the potential energy function, for a sufficiently 'strong' topology change in the Σ_v 's or the M_v 's at some v_c might induce a phase transition at a temperature such that $v_c = \frac{1}{N} \langle V \rangle$ because, as we have just seen, at very large N the measure concentrates on a single 'slice'.

An important remark is in order. All these results can be reformulated considering the submanifolds $M_v = \{q \in M | V(q) \leq Nv\}$ instead of the Σ_v 's; the relation between these two families of submanifolds is $\Sigma_v = \partial M_v$. The reason for the possibility of substituting the M_v 's to the Σ_v 's is in the fact that the Liouville measure of M_v is the same as that of Σ_v when $N \to \infty$, and that topology changes of the Σ_v 's do occur simultaneously with those in the M_v 's apart from very particular cases. In applications, using the M_v 's instead of the Σ_v 's may

⁴ This holds at least for systems with short-ranged interactions, but also in many systems where interactions are extensive even if not additive like some mean-field models.

be easier (for instance, in some cases Morse theory allows a direct calculation of the topology changes in the M_v 's using the potential energy as a Morse function [12, 13]).

As already noted in section 1, the idea of the topological hypothesis has been discussed and tested in some particular models, and a theorem has been proven showing that—for a wide class of systems—topology changes in the Σ_v 's are a necessary condition for a phase transition to occur [20]. In the following section we are going to show how a *sufficient* condition can be derived in the case of the spontaneous breaking of a \mathbb{Z}_2 symmetry.

3. Sufficient topological condition for \mathbb{Z}_2 -symmetry breaking

Let us now consider a system of the class (7) with a potential energy which is \mathbb{Z}_2 -invariant. As we have shown in the previous section, in the thermodynamic limit the canonical ensemble average of a function of the coordinates is given by equation (18). Let us now consider, instead of a generic function A(q), a function whose average is a order parameter for the \mathbb{Z}_2 -symmetry breaking, i.e.,

$$A(q) = \frac{1}{N} \sum_{i=1}^{N} q_i.$$
 (20)

By inserting equation (20) into equation (18), at a first sight we are led to conclude that no symmetry breaking is possible also in the thermodynamic limit, because all the hypersurfaces Σ_v , being level sets of the potential energy function V, must have all the symmetry of the function V itself, and in particular the \mathbb{Z}_2 symmetry; hence⁵ the order parameter is zero for any value of T.

This conclusion is wrong. The Σ_v 's may be composed of two or more disjoint connected components, and although the whole Σ_v must respect the invariance, each single connected component need not to be \mathbb{Z}_2 -invariant: each one may be the image of another one under the symmetry operation. If Σ_v is made up of disjoint connected components, then the definition (18) of the ensemble average is perfectly legitimate, but cannot be consistent with the actual behaviour of the system, because the representative point of the system can explore only one of the connected components. This may be easily seen if we think of the dynamics. Saying that when $N \to \infty$ the support of the measure is $\Sigma_{\overline{v}(\beta)}$ is equivalent to saying that the measure is formally the standard Boltzmann weight

$$\varrho_{\infty}(q;\beta) = \frac{1}{Z_{\infty}} e^{-\beta V_{\infty}(q;\beta)}$$
(21)

with effective potential V_{∞} given by

$$V_{\infty}(q;\beta) = \begin{cases} Nv & \text{if } q \in \Sigma_{\overline{v}(\beta)}, \\ +\infty & \text{if } q \in M \setminus \Sigma_{\overline{v}(\beta)}, \end{cases}$$
 (22)

at t=0, the system will be in one of the disjoint components, and it will remain there forever: it can never jump to another one because this would require to jump over an infinite energy barrier. Hence, if $\Sigma_v = \Sigma_v^1 \cup \Sigma_v^2 \cup \cdots \cup \Sigma_v^n$ with $\Sigma_v^a \cap \Sigma_v^b = \varnothing \forall a, b$, the restricted ensemble average being equal to a time average will be given by one of the following

$$\langle A \rangle^{a}(\beta) \underset{N \to \infty}{\longrightarrow} = \frac{1}{\tilde{Z}^{a}(\beta)} \int_{\Sigma_{\overline{v}(\beta)}^{a}} \frac{A|_{\Sigma^{a}} d\Sigma}{\|\nabla V\|}, \qquad a = 1, \dots, n,$$
 (23)

⁵ We are implicitly assuming that also the integration measure $d\Sigma/\|\nabla V\|$ in equation (18) is still \mathbb{Z}_2 -invariant in the thermodynamic limit; this is perfectly reasonable because if V(q) is \mathbb{Z}_2 -invariant, $\|\nabla V\|$ is \mathbb{Z}_2 -invariant too. However, since it is not a uniform measure, there may be particular cases in which it concentrates on submanifolds of Σ_v , and this may imply the possibility of a symmetry breaking: we will discuss this case in the following.

where the correct value of a will be specified by the initial conditions, and

$$\tilde{Z}^{a}(\beta) = \int_{\Sigma_{\pi(\alpha)}^{a}} \frac{\mathrm{d}\Sigma}{\|\nabla V\|}, \qquad a = 1, \dots, n.$$
 (24)

If neither Σ_v^a nor A(q) are \mathbb{Z}_2 -invariant, definitions (18) and (23) do not yield the same result; in particular, the average of $\frac{1}{N}\sum_{i=1}^N q_i$ according to equation (23) may give a nonzero result, so that symmetry breaking is possible.

We note that the disjoint connected components Σ_v^a of Σ_v play a role analogous to that of pure states in the standard approach to the formal treatment of symmetry breaking [22, 26], while their union (i.e., the whole Σ_v) plays the role of the mixed state.

We can now state the following theorem.

Theorem 1 (sufficient topological condition for \mathbb{Z}_2 -symmetry breaking). Let us consider a system of the class (7) with N degrees of freedom and a potential energy V bounded below which is \mathbb{Z}_2 -invariant. Let the entropy per degree of freedom be well defined in the thermodynamic limit, i.e., the function a(v) defined in equation (14) exist and be continuous and piecewise differentiable. Let Σ_v be the family of equipotential hypersurfaces of the configuration space M defined as in equation (10). Without loss of generality, let $\min(V) = 0$. Let $v'' > v' \geqslant 0$ be two values of the potential energy per degree of freedom V/N such that $\Sigma_v = \bigcup_{a=1}^n \Sigma_v^a \ \forall v \in (v', v'')$, with $\Sigma_v^a \cap \Sigma_v^b = \varnothing \ \forall a, b,$ and such that $\forall a \ \exists b \neq a : \mathcal{Z}(\Sigma_v^a) = \Sigma_v^b$ where \mathcal{Z} is the \mathbb{Z}_2 -symmetry map on M, $\mathcal{Z}(q) = -q$.

Then, in the thermodynamic limit the \mathbb{Z}_2 symmetry is spontaneously broken for all the temperatures $T \in (T', T'')$, where $T'' > T' \geqslant 0$.

Proof. Thanks to the hypotheses on the function a(v), the statistical average of the potential energy per degree of freedom, $\overline{v}(T)$, is given by equation (17) and is monotonically increasing as T is varied from 0 to $+\infty$, because $\frac{d\overline{v}}{dT} < 0$ would imply a negative (configurational) heat capacity, which is forbidden in the canonical ensemble [25]. Then there exists $T', T'' \geq 0, T' = \overline{v}^{-1}(v'), T'' = \overline{v}^{-1}(v'')$, such that $\overline{v}(T) \in (v', v'') \, \forall T \in (T', T'')$. For the sake of clarity let us assume that for $v \in (v', v'')$ the equipotential hypersurface is made up only of two disjoint connected components, $\Sigma_v = \Sigma_v^+ \cup \Sigma_v^- \, \forall v < v'$, with $\Sigma_v^+ \cap \Sigma_v^- = \emptyset$ and $\mathcal{Z}(\Sigma_v^+) = \Sigma_v^-$; the extension to a larger number of components is straightforward. According to equation (23), for $T \in (T', T'')$ the order parameter is

$$m^{\pm} = \left\langle \frac{1}{N} \sum_{i=1}^{N} q_i \right\rangle^{\pm} \xrightarrow[N \to \infty]{} = \frac{1}{N \tilde{Z}^{\pm}} \int_{\Sigma_{\tau(\beta)}^{\pm}} \frac{\sum_{i=1}^{N} q_i \, \mathrm{d}\Sigma}{\|\nabla V\|}, \tag{25}$$

and since the integrand is odd under $\mathcal{Z}, \tilde{Z}^+ = \tilde{Z}^-$ —this follows from the definition in equation (24)—and $\mathcal{Z}(\Sigma_v^+) = \Sigma_v^-$ we have

$$m^{+} = -m^{-} \neq 0, \tag{26}$$

because in order to have $m^{\pm}=0$ each of the Σ_{v}^{\pm} 's should be symmetric around q=0, but this is impossible if they are disconnected and \mathbb{Z}_{2} -invariant. Then the symmetry is spontaneously broken when $T\leqslant T'$.

Corollary 1. Let us consider a system of the class (7) with N degrees of freedom and a potential energy V bounded below which is \mathbb{Z}_2 -invariant, an let it have two degenerate distinct absolute minima $q^+ = -q^-$ whose value is $\min(V) = 0$. Let the entropy per degree of freedom exist as in theorem 1. Let Let v' > 0 be a value of the potential energy per degree of freedom V/N such that all the Σ_v 's are homeomorphic for v < v'.

Then, in the thermodynamic limit the \mathbb{Z}_2 symmetry is spontaneously broken for all the temperatures smaller than a finite value T'.

Proof. When $v \to 0$, $\Sigma_v = \Sigma_v^+ \cup \Sigma_v^-$, where Σ_v^\pm are homeomorphic to (N-1)-spheres and $\Sigma_v^+ \cap \Sigma_v^- = \varnothing$. Since no topology change occurs until v', for all the temperatures smaller than $T' = \overline{v}^{-1}(v')$ we are in the situation of theorem 1, whence the thesis.

We note that the crucial ingredient to obtain the sufficient condition of theorem 1 is that the value of the potential energy below which the topology of the Σ_v 's is such that they are made up of disjoint connected components must be proportional to N, and this agrees with the qualitative reasoning of section 2.1. Being a sufficient condition, but not a necessary one, this obviously does not rule out the possibility of having a symmetry breaking with less strong assumptions. Moreover, we have proven that the symmetry is broken below T'', but neither that it is restored above T'', nor that there is a phase transition at T'' or at any other T. To prove that, we have to strengthen the hypotheses, as in the following.

Theorem 2 (sufficient condition for \mathbb{Z}_2 -symmetry-breaking phase transitions). In addition to the hypotheses of theorem1, let $v''' \geqslant v''$ be a value of the potential energy per degree of freedom V/N such that Σ_v is made of a single connected component for v > v'''. Let also the support of the canonical measure be the whole $\Sigma_{\overline{v}(T)}$ when $\overline{v}(T) \geqslant v'''$ also in the thermodynamic limit.

Then, in the thermodynamic limit there exist finite temperatures $T' < T'' \leqslant T'''$ such that the \mathbb{Z}_2 symmetry is spontaneously broken for all $T \in (T', T'')$ and is restored for all $T \geqslant T'''$. There is also at least a phase transition (or more than one) at T_c such that $T'' \leqslant T_c \leqslant T'''$. If $v'' = v''' = v_c$, then there is just one phase transition at $T_c = \overline{v}^{-1}(v_c)$.

Proof. Theorem 1 ensures that $m \neq 0$ for $T \in (T', T'') = (\overline{v}^{-1}(v'), \overline{v}^{-1}(v''))$. Then, reasoning as in the proof of theorem 1, there exists T''' > 0, $T''' = \overline{v}^{-1}(v''')$ such that $\overline{v}(T) \geqslant v''' \ \forall T \geqslant T'''$. Then, for $T \geqslant T'''$ the order parameter is

$$m = \left\langle \frac{1}{N} \sum_{i=1}^{N} q_i \right\rangle \underset{N \to \infty}{\longrightarrow} = \frac{1}{NZ} \int_{\Sigma_{\overline{v}(\beta)}} \frac{\sum_{i=1}^{N} q_i \, \mathrm{d}\Sigma}{\|\nabla V\|} = 0, \tag{27}$$

because the $\Sigma_{\overline{v}(\beta)}$'s are all symmetric: the symmetry is restored. Hence, the order parameter m is nonzero when $T \in (T', T'')$, and is constant and equal to zero when T > T'''. Then the function m(T) has at least a non-analytic point for a temperature $T'' < T_c < T'''$; thus there is at least one phase transition in the system. If $v'' = v''' = v_c$, then there is a transition occurring at $T_c = \overline{v}^{-1}(v_c)$.

We note that the hypothesis that the support of the measure remains the whole $\Sigma_{\overline{v}(T)}$ when $\overline{v}(T)\geqslant v'''$ also in the thermodynamic limit is essential, because without this assumption we cannot prove that m=0. If as $N\to\infty$ the support of the measure shrinks to a submanifold of $\Sigma_{\overline{v}(T)}$, then the symmetry may remain broken even if $\Sigma_{\overline{v}(T)}$ is \mathbb{Z}_2 -symmetric. We believe that this case is not a purely academic one: it is probably what happens in at least one physically relevant example (the mean-field φ^4 model, see section 5). This assumption was not necessary at all in proving theorem 1, because this may affect only the actual value of m, but not the fact that it is nonzero.

These two theorems have rather strong assumptions, which may probably be weakened. Moreover, for a generic many-particle system it is not an easy task at all to characterize all the topology changes undergone by the Σ_{ν} 's (see e.g. the discussion given in [7, 12, 13]), so that we are not claiming to have derived a practical all-purpose method to prove the existence of

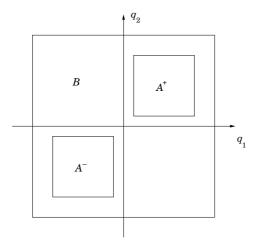


Figure 1. Sketch of the hypercubes A^{\pm} and B for N=2.

symmetry-breaking phase transitions in generic systems. Nonetheless, the theorems do allow one to make predictions, which are confirmed by the analysis of some known models, to be discussed in section 5. But before doing that, let us discuss an abstract toy model we introduce in the next section, whose main purpose is to illustrate the theorems in a simple and clear way, but which may have also some interest on its own.

4. Hypercubic model

We now introduce and solve an abstract model to enlighten, in a pedagogical way, the content of the theorems proven in the last section. This model is rather abstract, and from a physical point of view it can be seen as a model of a particle bouncing in a potential in an N-dimensional space, but we build it starting directly with the equipotential hypersurfaces Σ_v .

The simplest \mathbb{Z}_2 -invariant potential is a double square well in one dimension, i.e.,

$$V(q) = \begin{cases} 0 & \text{if } a < |q| < b, \\ v_0 & \text{if } a > |q|, \\ +\infty & \text{if } |q| > b, \end{cases}$$

$$(28)$$

with 0 < a < b. In this simple case the configuration space M is just the real line \mathbb{R} . Our first toy model, which we will refer to as the hypercubic model, is nothing but a generalization to N dimensions of this double square well. The configuration space is now \mathbb{R}^N , and in M we consider two disjoint hypercubes A^+ and A^- , symmetric under \mathbb{Z}_2 , and a third hypercube B, centred in the origin, such that A^+ , $A^- \subset B$. Then we define

$$V(q) = \begin{cases} 0 & \text{if } q \in A^{\pm}, \\ Nv_c & \text{if } q \in B \setminus \{A^+ \cup A^-\}, \\ +\infty & \text{if } q \in \mathbb{R}^N \setminus B. \end{cases}$$
 (29)

This potential is \mathbb{Z}_2 -invariant by construction. The hypercubes A^{\pm} and B are sketched in figure 1 in the case N=2.

The equipotential hypersurfaces Σ_v are then

$$\Sigma_{v} = \begin{cases} \varnothing & \text{if } v < 0, \\ A^{+} \cup A^{-} & \text{if } v = 0, \\ \varnothing & \text{if } 0 < v < v_{c}, \\ B \setminus \{A^{+} \cup A^{-}\} & \text{if } v = v_{c}, \\ \varnothing & \text{if } v > v_{c}. \end{cases}$$

$$(30)$$

Then the topology of the Σ_{v} 's is such that (\sim stands for 'is homeomorphic to')

$$\Sigma_{v} \sim \begin{cases} \varnothing & \text{if} \quad v < 0, \\ D^{N} + D^{N} & \text{if} \quad v = 0, \\ \varnothing & \text{if} \quad 0 < v < v_{c}, \\ D_{2}^{N} & \text{if} \quad v = v_{c}, \\ \varnothing & \text{if} \quad v > v_{c}. \end{cases}$$

$$(31)$$

where D^N is a disc in \mathbb{R}^N , with D_2^N we denote a two-punctuated disc (a disc with two disjoint discs removed) and '+' stands for the disjoint union. The fact that apart from the values v=0 and $v=v_c$ the Σ_v 's are empty sets is due to the very singular nature of the potential, which has only two possible values instead of a continuous interval: as v increases starting from values smaller than zero, the system potential energy actually 'skips over' all the values but 0 and v_c , because these are the only allowed values of V/N. Nonetheless, we see that the Σ_v 's of the hypercubic model undergo a topology change as v changes from v=0 to $v=v_c$ of the kind described in theorem 2, in the case $v'=v''=v_c$. However, the situation is much clearer if we consider the M_v manifolds instead of the Σ_v 's: we have

$$M_{v} = \begin{cases} \varnothing & \text{if} \quad v < 0, \\ A^{+} \cup A^{-} & \text{if} \quad 0 \leq v < v_{c}, \\ B & \text{if} \quad v \geqslant v_{c}, \end{cases}$$

$$(32)$$

and the topology of the M_v 's is

$$M_{v} \sim \begin{cases} \varnothing & \text{if} \quad v < 0, \\ D^{N} + D^{N} & \text{if} \quad 0 \leq v < v_{c}, \\ D^{N} & \text{if} \quad v \geqslant v_{c}. \end{cases}$$

$$(33)$$

Then the M_v 's of the hypercubic model undergo a topology change as v changes from v=0 to $v=v_c$ precisely of the kind described in theorem 2, in the case $v'=v''=v_c$, and theorem 2 (applied to the M_v 's) states that the hypercubic model, in the thermodynamic limit $N\to\infty$, undergoes a phase transition with \mathbb{Z}_2 -symmetry breaking at a finite temperature T_c such that $\frac{1}{N}\langle V\rangle(T_c)=v_c$. Let us see it explicitly, solving the model.

At any finite N, the configurational partition function of the hypercubic model is

$$Z_N(\beta) = \int_{\mathbb{R}^N} d^N q \, e^{-\beta V(q)} = \int_{A^+} d^N q + \int_{A^-} d^N q + e^{-\beta N v_c} \int_{B \setminus \{A^+ \cup A^-\}} d^N q$$
 (34)

and denoting by a and b the length of the side of A^{\pm} and B, respectively, we obtain

$$Z_N(\beta) = 2a^N + (b^N - 2a^N) e^{-\beta N v_c},$$
(35)

where $b \ge 2a$ because A^+ , $A^- \subset B$. Thermodynamic functions can then be computed at any finite N and their limit as $N \to \infty$ can be studied directly. We shall see that in the following, but before doing that we note that when N is large we can write

$$Z_N(\beta) \underset{N \to \infty}{\longrightarrow} 2a^N + b^N e^{-\beta N v_c} = 2 e^{N \log a} + e^{N(\log b - \beta v_c)}, \tag{36}$$

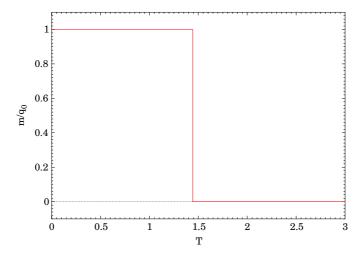


Figure 2. Order parameter of the hypercubic model in the thermodynamic limit, as a function of T. Here $v_c = 1$, a = 1, b = 2a, so that $T_c = (\log 2)^{-1}$. Only the positive branch is plotted.

so that in the thermodynamic limit only the largest of the two exponentials contributes to Z, and there will be a critical value β_c of the inverse temperature β , given by the equation

$$\log a = \log b - \beta_c v_c \tag{37}$$

whose solution is

$$\beta_c = \frac{1}{v_c} \log \left(\frac{b}{a} \right),\tag{38}$$

such that

$$Z_{N}(\beta) \underset{N \to \infty}{\longrightarrow} \begin{cases} 2e^{N \log a} & \text{if } \beta > \beta_{c}, \\ e^{N(\log b - \beta v_{c})} & \text{if } \beta < \beta_{c}. \end{cases}$$
(39)

This means that the system feels an effective double-well potential, with potential energy zero and the two wells separated by an infinite barrier, for $\beta > \beta_c$ and an effective single well, symmetric potential with potential energy v_c when $\beta < \beta_c$. Hence the symmetry is broken when $\beta > \beta_c$. The value of the order parameter

$$m = \frac{1}{N} \left\langle \sum_{i=1}^{N} q_i \right\rangle,\tag{40}$$

where the average is the restricted one when the symmetry is broken, will be, in the thermodynamic limit,

$$m(\beta) = \begin{cases} \pm q_0 & \text{if } \beta > \beta_c, \\ 0 & \text{if } \beta < \beta_c, \end{cases}$$

$$\tag{41}$$

where q_0 is the value of all the coordinates q_1, \ldots, q_N of the centre of the A^+ hypercube. The order parameter is plotted as a function of $T = \beta^{-1}$ in figure 2. In the same limit, the average potential energy per degree of freedom will be

$$\langle v \rangle (\beta) = -\frac{1}{N} \frac{\partial}{\partial \beta} \log Z_N(\beta) = \begin{cases} 0 & \text{if } \beta > \beta_c, \\ v_c & \text{if } \beta < \beta_c, \end{cases}$$
(42)

so that the phase transition is a discontinuous (first-order) one

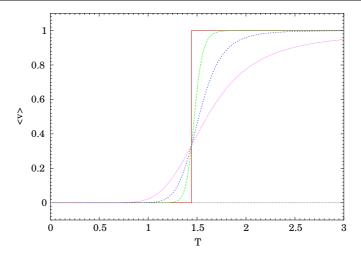


Figure 3. Average potential energy of the hypercubic model as a function of T. The different smooth curves are the finite-N result (43) with N=10, 20 and 50, while the piecewise constant curve is the $N\to\infty$ limit (42). Numerical values as in figure 2.

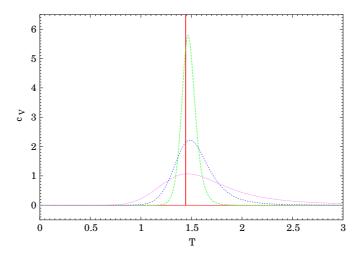


Figure 4. As in figure 3 for the specific heat c_V .

Computing the thermodynamic functions at finite N one finds for the average potential energy per degree of freedom

$$\langle v \rangle (\beta; N) = \frac{v_c(b^N - 2a^N) e^{-\beta N v_c}}{2a^N + (b^N - 2a^N) e^{-\beta N v_c}},$$
(43)

and for the configurational specific heat

$$c_V(\beta; N) = \frac{2N\beta^2 v_c^2 a^N (b^N - 2a^N) e^{-\beta N v_c}}{[2a^N + (b^N - 2a^N) e^{-\beta N v_c}]^2}.$$
 (44)

These functions are plotted in figures 3 and 4. We see that at any finite N both $\langle v \rangle$ and c_V are regular functions, which converge (nonuniformly) to the limiting non-analytic functions already determined before. As to the specific heat, since $\langle v \rangle$ is a piecewise constant function in the thermodynamic limit, $c_V = 0$ everywhere but at T_c where it has a δ -like singularity.

The hypercubic model is undoubtedly very abstract, for it describes a particle in an *N*-dimensional potential which is highly singular: yet it is extremely simple and neatly illustrates some consequences of theorem 2. Moreover, it can be probably considered as one of the most elementary models exhibiting a phase transition, so that it has a pedagogical interest on its own.

However, as we shall see in the next section, there are models, already known in the literature, which can be analysed in terms of the theorems of section 3, and whose potential energy function is indeed regular and describes the interaction among microscopic degrees of freedom, although in a not completely realistic way due to its mean-field character.

5. Physical models

5.1. Mean-field spherical model

A physical example which can be exactly analysed in terms of theorem 2 is the mean-field spherical model, recently studied in [14, 27], which is the mean-field version of the model originally introduced by Kac and Berlin in 1952 [28]. It is an Ising-like system with continuous variables: the potential energy is

$$V(\varphi) = -\frac{1}{2N} \sum_{i,j=1}^{N} \varphi_i \varphi_j, \tag{45}$$

where the variables $\varphi_i \in \mathbb{R}$, i = 1, ..., N, are subject to the condition

$$\sum_{i=1}^{N} \varphi_i^2 = N \tag{46}$$

which constraints the variables to live on the (N-1)-dimensional sphere of radius \sqrt{N} centred in the origin of \mathbb{R}^N , whence the name 'spherical model'. The \mathbb{Z}_2 invariance of the potential is apparent from equation (45). The potential energy is also bounded, so that the potential energy per degree of freedom is bounded too: $v \in \left[-\frac{1}{2}, 0\right]$.

The topology of the equipotential hypersurfaces Σ_v of the mean-field spherical model can be easily determined, and one finds [14, 27] that

$$\Sigma_{v} \sim \begin{cases} \emptyset & \text{if } v < -\frac{1}{2}, \\ \mathbb{S}^{N-2} + \mathbb{S}^{N-2} & \text{if } -\frac{1}{2} < v < 0, \\ \mathbb{S}^{N-2} & \text{if } v = 0. \end{cases}$$
(47)

We are in the situation described in theorem 2, which then predicts that this model, in the canonical ensemble, has a phase transition with \mathbb{Z}_2 -symmetry breaking at a finite temperature T_c such that $\langle v \rangle (T_c) = 0$. This is indeed what happens, and the critical temperature turns out to be $T_c = 1$ [14].

The mean-field spherical model is thus a nice illustration of the consequences of theorem 2.

5.2. Mean-field φ^4 model

An example where theorem 1 holds is provided by another mean-field version of a continuousspin Ising model, the mean-field φ^4 model [17–19]. The interaction potential is

$$V(\varphi) = \frac{J}{N} \sum_{i,j=1}^{N} \varphi_i \varphi_j + \sum_{i=1}^{N} \left(-\frac{1}{2} \varphi_i^2 + \frac{1}{4} \varphi_i^4 \right), \tag{48}$$

where J>0 is a coupling constant and $\varphi_i\in\mathbb{R},\,i=1,\ldots,N$. Again the \mathbb{Z}_2 symmetry is apparent from equation (48); this potential is bounded below, but not above, and $v\in[v_{\min},+\infty)$, where $v_{\min}=-\frac{(J+1)^2}{4}$. There are two equivalent distinct minima, $\varphi_i=\pm\sqrt{J+1}$, $i=1,\ldots,N$, then as $v\to v_{\min}$

$$\Sigma_n \sim \mathbb{S}^{N-1} + \mathbb{S}^{N-1}. \tag{49}$$

It has been numerically shown [17] that for any N and any J>0 there are no topology changes⁶ in the Σ_v 's as long as < v', where v'<0 is a finite value which grows when J grows. Then, this model fulfils the hypotheses of theorem 1, or more precisely those of corollary 1, so that the \mathbb{Z}_2 symmetry must be broken below a finite temperature $T'=\overline{v}^{-1}(v')$. This is precisely what happens: the magnetization m(T), which can be exactly calculated in the thermodynamic limit due to the mean-field character of the model, is nonzero for T< T'. For instance, as $J=\frac{1}{2}$, $v'\simeq -0.35$ and $T'\simeq 0.3$, while the critical temperature below which the symmetry is broken is $T_c\simeq 0.4$; when J=1, $v'\simeq -0.25$ and $T'\simeq 0.9$, while $T_c\simeq 1$ [17].

However, as v > 0, it has also been shown [17–19] that

$$\Sigma_{v} \sim \mathbb{S}^{N-1},$$
 (50)

but at least for sufficiently large values of J the \mathbb{Z}_2 symmetry remains broken also for temperatures $T > T'' = \overline{v}^{-1}(0)$. Then, although this model is a clear illustration of corollary 1, it does not behave as predicted by theorem 2, at variance with the mean-field spherical model. This means that at least one of the hypotheses of theorem 2 does not hold for the mean-field φ^4 model. As we will discuss elsewhere [29], in this case it is not true that the support of the equilibrium measure remains the whole $\Sigma_{\overline{v}}$ even in the thermodynamic limit, due to the additional constraint provided by the fact that the function whose average is the order parameter enters the potential⁷.

6. Concluding remarks

We have shown that the topological approach to phase transitions allows one to translate an intuitive, qualitative picture of the origin of discrete-symmetry-breaking phase transitions into a sufficient condition for such phenomenon to occur. This is a first step towards obtaining more general sufficient conditions for phase transitions, thus towards filling a gap in our present understanding of these ubiquitous and fascinating phenomena. The topological sufficient conditions have been derived here in the case of \mathbb{Z}_2 symmetry, but the proofs of theorems 1 and 2 are easily adaptable to more general discrete symmetries: we chose to restrict ourselves to \mathbb{Z}_2 for the sake of simplicity, and because of the great importance of this particular symmetry in the development of our understanding of the physics of phase transitions. We note that our sufficient conditions are not exclusively topological in nature, i.e., they cannot be formulated in terms of the topological properties of the $\Sigma'_v s$ alone: for example, we have also to introduce some hypotheses on the behaviour with N of the values of the energy at which some topology changes must happen. Nonetheless, these additional requirements appear absolutely natural,

⁶ More precisely, in [17] it has been shown that there are no topology changes in the manifolds M_v whose boundaries are the Σ_v 's, i.e., $\Sigma_v = \partial M_v$. Nonetheless, since $M_v \sim \mathbb{S}^N + \mathbb{S}^N$ as v < v' and $\partial \mathbb{S}^N = \mathbb{S}^{N-1}$, we have $\Sigma_v \sim \mathbb{S}^{N-1} + \mathbb{S}^{N-1}$ as v < v'.

⁷ This is true also for the spherical model and in other cases like the mean-field XY model [12]; nonetheless, in the latter cases V can be written as a function of the order parameter alone, so that even if it may restrict the support of the measure to a subset of the Σ_v , it cannot change its symmetry properties. Rigorously speaking, then, also for the mean-field spherical model one should say that theorem 2 holds even if its hypotheses may not be completely fulfilled.

and do not change the fact that the basic ingredient of the two theorems proven here comes from topology.

A simple model introduced here, the hypercubic model, and some mean-field models already known in the literature have been discussed in the light of these two theorems. It would obviously be particularly interesting to investigate some more realistic systems using these results. The natural candidate for such an investigation is the φ^4 model with short-range interactions in two or more dimensions. At present, only numerical results for the topology of the Σ_v 's are available for this model [10] which do not yet allow to state whether the hypotheses of some of the two theorems are fulfilled for this model. This is clearly one of the natural lines of development for future investigations.

We are aware that these sufficient conditions may well be not 'optimal' at all, in the sense that it may be possible to weaken the hypotheses; moreover, it is possible that in some cases the actual physical relevance of the particular phenomenon described here is small, because other mechanisms may be at work [30]. Nonetheless, the availability of a sufficiency criterion, although restricted to a particular class of transitions and maybe not optimal yet, opens also the possibility of using the topological approach to define phase transitions in finite systems, because the topology changes in the manifolds Σ_v which are at the basis of phase transitions do occur also in finite systems: work is in progress along this line. Moreover, the phenomenology of 'disconnection borders' found in some classical spin systems (see e.g. [31]) might be well related to our present results in the perspective of studying transitional phenomena in finite systems.

In conclusion, we believe that the present work adds some new insight to the topological approach to phase transitions, confirming its great potentialities.

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