Exact result on topology and phase transitions at any finite N

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We study analytically the topology of a family of submanifolds of the configuration space of the mean-field *XY* model, computing also a topological invariant (the Euler characteristic). We prove that a particular topological change of these submanifolds is connected to the phase transition of this system, and exists also at finite N. The present result is the first *analytic* proof that a phase transition has a topological origin and provides a key to a possible better understanding of the origin of phase transitions at their deepest level, as well as to a possible definition of phase transitions at finite N.

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Phase transitions (PTs) are one of the most striking phenomena in nature. They involve sudden qualitative physical changes, accompanied by sudden changes in the thermodynamic quantities measured in experiments. From a mathematical point of view, both qualitative and quantitative changes at PTs are conventionally described by the loss of analyticity of the probability measures and of the thermodynamic functions. According to statistical mechanics, such a nonanalytic behavior can exist only in the thermodynamic limit, i.e., in the case of a system with $N\to\infty$ degrees of freedom [1]. PTs in real systems would then be the "shadow," at finite but large N, of this idealized behavior. However, the necessity of taking the $N\to\infty$ limit to speak of PTs seems less satisfactory today, since there is growing experimental evidence of PT phenomena in systems with *small* N (e.g., atomic clusters, nuclei, and mesoscopic systems, in general [2]).

There is also another reason why the conventional approach to PTs is not yet completely satisfactory. Consider a classical system described by a Hamiltonian $\mathcal{H}=K(\pi)+V(\varphi)$, where $K(\pi)=1/2\Sigma^{N}_{i=1}\pi_i^2$ is the kinetic energy, $V(\varphi)$ is the potential energy and $\varphi\equiv\{\varphi_i\}$ and $\pi\equiv\{\pi_i\}$'s are, respectively, the canonical conjugate coordinates and momenta. Although, in principle, all the information on the statistical properties is contained in the function $V(\varphi)$, no general result is available to specify which features of $V(\varphi)$ are necessary and sufficient to entail the existence of a PT. This is the more surprising since in many cases, knowing *a priori* that a system undergoes a PT, several relevant properties of the PT can be predicted just in terms of very general features of $V(\varphi)$ (e.g., by means of renormalization-group techniques).

An alternative approach to PTs has been recently proposed [3–8], which connects the existence of a PT to the properties of the potential energy $V(\varphi)$, resorting to *topological* concepts. According to this topological hypothesis, PTs would be related to *topology changes* (TCs) of the submanifolds M_V of configuration space, defined by the potential energy $V(\varphi)$ as: $M_V=M_{E-K}$, i.e., the subsets of the configuration space M contained within the equipotential hypersurface of level $V=E-K$, where E is the total energy. In other words, the existence of a PT would be written in the potential energy function as the existence of a peculiar TC of the manifolds M_V. Abrupt TCs of these manifolds can yield singular derivatives in the microcanonical volume $\Omega(E)$ [9,10]; if this behavior is persistent with increasing N, such a TC will result in a loss of analyticity of the thermodynamic observables, only in the $N\to\infty$ limit [11].

The topological approach to phase transitions seems then very promising in the light of a possible solution to the two above-mentioned problems with the conventional approach to PTs, because not only does it link the existence of a PT with the analytical properties of the potential energy function $V(\varphi)$ encoding the topology of the M_V, independently of the statistical probability measures, but it also provides a natural way to extend the concept of a PT to finite N. In the topological approach, the loss of analyticity of the thermodynamic observables in the $N\to\infty$ limit is due to a deeper primitive topological cause of a PT, which is already present at finite N.

The topological approach has been put forward on a heuristic basis in Ref. [3]: since then, by means of numerical and analytical investigations on particular models, evidence has accumulated in favor of its validity, but this evidence is still circumstantial. For the lattice φ^4 model, indirect [4] as well as direct [6] evidence has been found, but only numerically. In Ref. [5], an analytical argument which strongly supports the validity of the topological approach in the case of the mean-field *XY* model has been given, however, it does not rigorously prove the existence of a TC which is connected to a PT. Moreover, these studies have shown that *not all* possible TCs are related to PTs [8], and no general argument is yet at hand to define the *sufficient* conditions under which a TC is actually related to a PT. Analytical, as well as numerical results [4–6], give no direct hint to the solution of this problem, suggesting only that a TC related to a PT should be a "second-order" one, i.e., not a mere change in the topology but also a "change in the way of changing" the topology. Confirmation or confutation of this idea, as well as further

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insight into the nature of the TCs related to PTs should be provided by analytical calculations of topological invariants of the manifolds M_V.

In the present paper, we prove on a firm mathematical basis the existence of a TC which is connected with the PT of the mean-field *XY* model. Moreover, we give a complete analytical characterization of all the TCs in the configuration space, which clearly indicates the difference between the TC related to the PT and other TCs. We are also able to compute analytically a topological invariant of the M_V, the Euler characteristic χ, showing that the TC connected to the PT corresponds here to a sharp discontinuous jump in χ. Incidentally this confirms that the TC related to the PT is "second-order" because also the derivative of χ shows a sharp change.

Although still limited to a particular model, the present result is the first analytical confirmation of the validity of the topological approach, which then can be put on a firm basis. Moreover, the technique here used to study analytically the TCs and to compute χ is completely general and could hopefully be applied also to other systems. To the best of our knowledge, this is also the first analytical calculation of the Euler characteristic for *N*-dimensional configuration spaces of physical models.

Let us now summarize a few needed facts about topology before discussing the case of our model. The TCs we are referring to are those transformations which map a manifold onto one which is not diffeomorphic to the previous one, i.e., which cannot be mapped back to it by means of a differentiable transformation. A TC is therefore any transformation which "breaks the fabric" of a manifold: making a hole—without boundary—in a sphere transforms it into a torus, and there is no smooth way to transform a torus back to a sphere. Morse theory [12] provides a way of classifying TCs of manifolds, and links *global* topological properties with *local* analytical properties of smooth functions defined on them, so that they can be used as a practical tool to study their topology. Given a (compact) *N*-dimensional manifold *M* and a smooth function *f*: $M \mapsto \mathbb{R}$, a point $\bar{x} \in M$ is called a *critical point* of *f* if $df=0$, i.e., if the differential of *f* at *x* vanishes, while the value $f(\bar{x})$ is called a *critical value*. A level set $f^{-1}(a)=\{x\in M: f(x)=a\}$ of *f* is called a *critical level* if *a* is a critical value of *f*, i.e., if there is at least one critical point $\bar{x}\in f^{-1}(a)$. The function *f* is called a *Morse function on M* if its critical points are all nondegenerate, i.e., if the Hessian of *f* at $\bar{x}$ has only nonzero eigenvalues, so that the critical points $\bar{x}$ are isolated. We now consider the configuration space of a classical system as our manifold *M*, and the potential energy per particle $\mathcal{V}(\varphi)=V(\varphi)/N$ as our Morse function. Then, the submanifolds M_v of *M* whose topology we want to investigate are

$$M_v=\mathcal{V}^{-1}(-\infty,v]=\{\varphi\in M:\mathcal{V}(\varphi)\leqslant v\}, \tag{1}$$

i.e., the same as the $M_V=M_{E-K}$ defined above (where in M_v, *V* has been rescaled by $1/N$, i.e., $v=V/N$, in order to make the comparison of systems with different *N* easier). All the submanifolds M_v of *M*, with increasing v, have the same topology until a critical level $\mathcal{V}^{-1}(\bar{v})$ is crossed. Here, the topology of M_v changes in a way completely determined by the local properties of the Morse function: at any critical level a *k*-handle $H^{(k)}$ is attached [13], where *k* is the *index* of the critical point, i.e., the number of negative eigenvalues of the Hessian matrix of $\mathcal{V}$ at this point. Notice that if there are $m>1$ critical points on the same critical level, with indices $k_1,\dots,k_m$, then the TC is made by attaching *m* disjoint handles $H^{(k_1)},\dots,H^{(k_m)}$. This way, by increasing v, the full configuration space *M* can be constructed sequentially from the M_v. Knowing the index of all the critical points below a given level v, we can obtain *exactly* the Euler characteristic of the manifolds M_v, given by

$$\chi(M_v)=\sum_{k=0}^{N}(-1)^k\mu_k(M_v), \tag{2}$$

where the *Morse number* μ_k is the number of critical points of $\mathcal{V}$ which have index *k* [15]. The Euler characteristic χ is a *topological invariant*: any change in $\chi(M_v)$ implies a TC in the M_v.

Thus, in order to detect and characterize topological changes in M_v, we have to find the critical points and the critical values of $\mathcal{V}$, which means solving the equations

$$\frac{\partial\mathcal{V}(\varphi)}{\partial\varphi_i}=0,\quad i=1,\dots,N, \tag{3}$$

and to compute the indices of *all* the critical points of $\mathcal{V}$, i.e., the number of negative eigenvalues of its Hessian

$$H_{ij}=\frac{\partial^2\mathcal{V}}{\partial\varphi_i\partial\varphi_j}\quad i,j=1,\dots,N. \tag{4}$$

In the case of the mean-field *XY* model, which describes a system of *N* equally coupled planar classical rotators [14], due to the mean-field character of the interactions, such a calculation can be done in a completely analytical way. This allows then a discussion of the relationship between TCs and the PT of this model, whose potential energy is

$$V(\varphi)=\frac{J}{2N}\sum_{i,j=1}^{N}[1-\cos(\varphi_i-\varphi_j)]-h\sum_{i=1}^{N}\cos\varphi_i, \tag{5}$$

where $\varphi_i\in[0,2\pi]$ is the rotation angle of the *i*th rotator and *h* is an external field. The model describes also a planar (*XY*) Heisenberg system with interactions of equal strength among all the classical spins $\mathbf{s}_i=(\cos\varphi_i,\sin\varphi_i)$. We consider only the ferromagnetic case $J>0$; for the sake of simplicity, we set $J=1$. In the limit $h\to 0$, the system has a continuous PT, with classical critical exponents, at $T_c=1/2$, or $\varepsilon_c=3/4$, where $\varepsilon=E/N$ is the total energy per particle [14]. Defining the magnetization vector per particle $\mathbf{m}=(m_x,m_y)$, where $m_x=1/N\Sigma^N_{i=1}\cos\varphi_i$, $m_y=1/N\Sigma^N_{i=1}\sin\varphi_i$, the potential energy *V* can be written as a function of $\mathbf{m}$ as

$$V(\varphi)=V(m_x,m_y)=\tfrac{N}{2}(1-m_x^2-m_y^2)-hNm_x. \tag{6}$$

The range of values of the potential energy per particle, $\mathcal{V}=V/N$, is then $-h\leqslant\mathcal{V}\leqslant 1/2+h^2/2$.

The configuration space M of the model is an N-dimensional torus, being parameterized by the N angles $\{\varphi_i\}=\varphi_1,\dots,\varphi_N$. We now study the topology of the family of submanifolds M_v for this model. First, since TCs of M_v can occur only at critical points of $\mathcal{V}$, there are no TCs when $v>1/2+h^2/2$, i.e., all the M_v's with $v>1/2+h^2/2$ must be diffeomorphic to the whole M, that is, they must be N tori. Then one has to find all the solutions of Eqs. (3), which can be rewritten in the form [5,8]

$$(m_x+h)\sin\varphi_i - m_y\cos\varphi_i = 0, \quad i=1,\dots,N. \tag{7}$$

As long as $(m_x+h)\neq 0$ and $m_y\neq 0$ (m_x and m_y are both zero only on the level $v=1/2+h^2/2$), the solutions of Eqs. (7) are all those configurations for which the angles φ_i are either 0 or π. These configurations correspond to a value of v which depends only on the number of angles n_π which are equal to π, and using Eq. (6) one obtains

$$v(n_\pi)=\frac{1}{2}\left[1-\frac{1}{N^2}(N-2n_\pi)^2\right]-\frac{h}{N}(N-2n_\pi), \tag{8}$$

where $0\leqslant n_\pi\leqslant N$. We have thus shown that as v changes from its minimum $-h$ (corresponding to $n_\pi=0$) to 1/2 (corresponding to $n_\pi=N/2$) the manifolds M_v undergo a sequence of topology changes at the N critical values $v(n_\pi)$ given by Eq. (8). There might be a TC also at the last (maximum) critical value $v_c=1/2+h^2/2$. However, the above argument does not prove it, since the critical points of $\mathcal{V}$ corresponding to this critical level may be degenerate [16], so that on this level, $\mathcal{V}$ would not be a proper Morse function. Then, a critical value v_c is still a necessary condition for the existence of a TC, but it is no longer sufficient. However, as argued in Refs. [5,8], it is just this TC at v_c which should be related to the thermodynamic PT of the mean-field XY model. For the temperature T, the energy per particle ε and the average potential energy per particle $u=\langle\mathcal{V}\rangle$ obey, in the thermodynamic limit, the equation $2\varepsilon=T+2u(T)$, where we have set Boltzmann's constant equal to one. Substituting in this equation the values of the critical energy per particle and of the critical temperature, we get $u_c=u(T_c)=1/2$; as $h\to 0$, $v_c\to 1/2$, so that $v_c=u_c$. Thus, a TC in M occurring at this v_c, where v_c is *independent* of N, is connected with the PT in the limit $N\to\infty$, and $h\to 0$, when indeed thermodynamic PTs are usually defined.

Let us now prove that a TC at v_c actually exists and try to understand why it is different from the other TCs, i.e., those occurring at $0\leqslant v<v_c$. To do that, we characterize all the TCs occurring at the critical values $0\leqslant v<v_c$ using Morse theory, computing the *indices* of the critical points of $\mathcal{V}$. At these points, where the angles are either 0 or π, we can write the Hessian matrix (4) in the form $NH=D+B$, where D is diagonal, $D=\mathrm{diag}(\delta_i)$, with $\delta_i=(m_x+h)\cos\varphi_i$, and the elements of B, b_{ij}, can be written in terms of a vector σ whose N elements are either 1 or -1: $b_{ij}=-1/N\sigma_i\sigma_j$, with $\sigma_i=+1$ (resp. -1) if $\varphi_i=0$ (resp. π). The matrix B has only one nonzero eigenvalue. This implies that the number of negative eigenvalues of H equals the number of negative eigenvalues of $D\pm 1$ [17], so that as N gets large, we can conveniently approximate the index of the critical point with the number of negative δ's at x. At a given critical point, with given n_π, the eigenvalues of D are

$$\delta_i=m_x+h \quad i=1,\dots,N-n_\pi; \tag{9a}$$

$$\delta_i=-(m_x+h) \quad i=N-n_\pi+1,\dots,N, \tag{9b}$$

where the x component of the magnetization vector is $m_x=1-2n_\pi/N$, so that $m_x>0$ (resp. <0) if $n_\pi\leqslant N/2$ (resp. $>N/2$). Then, if the external field h is sufficiently small, and denoting by index (n_π) the index of a critical point with given n_π, we can write

$$\mathrm{index}(n_\pi)=n_\pi \qquad \text{if } n_\pi\leqslant\frac{N}{2}, \tag{10a}$$

$$\mathrm{index}(n_\pi)=N-n_\pi \quad \text{if } n_\pi>\frac{N}{2}. \tag{10b}$$

The number $C(n_\pi)$ of critical points having a given n_π, which is the number of distinct strings of 0's and π's of length N having n_π occurrences of π, is given by the binomial coefficient $C(n_\pi)=\binom{N}{n_\pi}$. Thus, at any critical level $-h\leqslant v(n_\pi)\leqslant 1/2$, where $v(n_\pi)$ is given by Eq. (8), a topological change in M_v occurs, which is made up of attaching $C(n_\pi)$ k handles, where $k(n_\pi)=$ index (n_π) given in Eq. (10). Here, n_π as a function of v can be obtained by solving Eq. (8), yielding

$$n_\pi^{(+)}(v)=\mathrm{int.}\left\{\frac{N}{2}\left[1+h\pm\sqrt{h^2-2\left(v-\frac{1}{2}\right)}\right]\right\}, \tag{11}$$

where int.$\{a\}$ stands for the integer part of a. Equations (10) and (11) allow us to write the Morse numbers μ_k of the manifolds M_v, for $-h\leqslant v<1/2+h^2/2$, as

$$\mu_k(v)=\{1-\Theta[k-n_\pi^{(-)}(v)]+\Theta[N-k-n_\pi^{(+)}(v)]\}\times\binom{N}{k}, \quad k=0,1,\dots,N, \tag{12}$$

where $\Theta(x)$ is the Heaviside theta function. We note that since $0\leqslant n_\pi^{(-)}\leqslant N/2$ and $N/2+1\leqslant n_\pi^{(+)}\leqslant N$, Eq. (12) implies $\mu_k(v)=0\ \forall k>N/2$, i.e., *no critical points with index larger than* $N/2$ *exist as long as* $v<1/2+h^2/2$. On the other hand, for $v>1/2+h^2/2$, M_v must be an N-torus $\mathbb{T}^N$, and for *any* Morse function on such a manifold, one has [18] $\mu_k(\mathbb{T}^N)\geqslant\binom{N}{k}$ for $k=0,1,\dots,N$. Thus, as $1/2\leqslant v<1/2+h^2/2$, the manifold is only "half" an N torus, and since we know that for $v>1/2+h^2/2$, M_v is an N torus, we conclude that at $v=v_c=1/2+h^2/2$, a TC *must* occur, which involves the attaching of $\binom{N}{k}$ k handles for each k ranging from $N/2+1$ to N. This is surely a "big" TC: all of a sudden, "half" an N torus becomes a full N torus. Now we can use Eqs. (2), (11), and (12) to compute the numerical values of the Euler characteristic of the manifolds M_v as a function of v: it turns out that χ jumps from positive to negative values, so that it is easier to look at $|\chi|$. In Figure 1, $\log(|\chi|(M_v))/N$ is plotted as

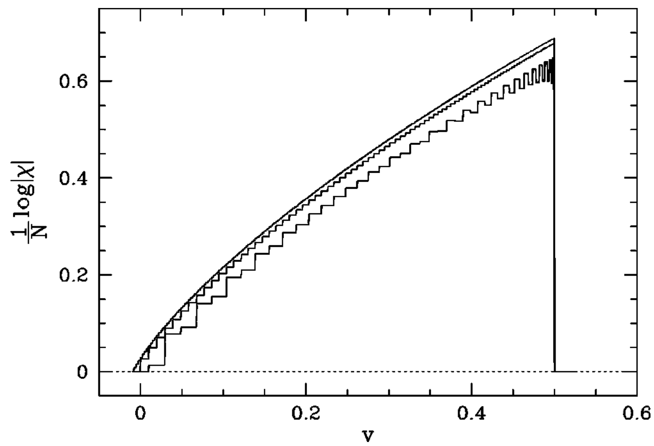

FIG. 1. Plot of $\log(|\chi|(M_v))/N$ as a function of v for $h=0.01$ and increasing $N=50$, 200, 800 (from bottom to top).

a function of v for various values of N ranging from 50–800. The ''big'' TC occurring at the maximum value v_c of $\mathcal{V}$, which corresponds in the thermodynamic limit to the PT, implies a discontinuity of $|\chi|$, jumping from a big value [$\mathcal{O}(e^N)$ in our case] to zero, which is the value of χ for an N torus.

The analytical results we have presented provide analytical proof of the soundness of the topological approach to PTs as well as a possible hint about what could be the *sufficient* conditions for a TC in configuration space to yield a PT. For, in the model studied here, the N TCs which are not related to the PT involve the simultaneous attachment of handles which are all of the *same* type, while that occurring at v_c is the simultaneous attaching of handles of $\mathcal{O}(N)$ *different* types. Hence, we might *conjecture* that this is a sufficient condition for a TC to be in one-to-one correspondence with a thermodynamical PT, also in other models. The model studied here has nonphysical long-range interactions. However, since a cuspy pattern of the Euler characteristic—of the equipotential hypersufaces—was numerically found at the PT point also in the $2d$-lattice φ^4 model with nearest-neighbor interactions [6], we surmise that the results of the present paper may be of general validity; moreover, being analytic, they may provide the basis for a theory of the origin of PTs based on the topology of configuration space as encoded in the potential energy. The topological approach might also prove useful in dealing with some aspects of disordered systems such as glasses. In fact, for glass-forming liquids, topological concepts have been recently invoked [19].

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[16] The solutions of the two equations in N variables $m_x=m_y=0$ need not be isolated.

[17] The proof, to be published in a subsequent paper, follows from a theorem found in J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Clarendon, Oxford, 1965).

[18] The μ_k's are upper limits of the Betti numbers (see [15]); the kth Betti number of an N torus is $\binom{N}{k}$.

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