Journal of Statistical Physics, Vol. 111, Nos. 5/6, June 2003 (© 2003)

Phase Transitions and Topology Changes in Configuration Space

Lapo Casetti,[1] Marco Pettini,[2] and E. G. D. Cohen[3]

Received March 25, 2002; accepted December 23, 2002

The relation between thermodynamic phase transitions in classical systems and topological changes in their configuration space is discussed for two physical models and contains the first *exact analytic* computation of a topologic invariant (the Euler characteristic) of certain submanifolds in the configuration space of two physical models. The models are the mean-field XY model and the one-dimensional XY model with nearest-neighbor interactions. The former model undergoes a second-order phase transition at a finite critical temperature while the latter has no phase transitions. The computation of this topologic invariant is performed within the framework of Morse theory. In both models topology changes in configuration space are present as the potential energy is varied; however, in the mean-field model there is a particularly "strong" topology change, corresponding to a big jump in the Euler characteristic, connected with the phase transition, which is absent in the one-dimensional model with no phase transition. The comparison between the two models has two major consequences: (i) it lends new and strong support to a recently proposed topological approach to the study of phase transitions; (ii) it allows us to conjecture which particular topology changes could entail a phase transition in general. We also discuss a simplified illustrative model of the topology changes connected to phase transitions using of two-dimensional surfaces, and a possible direct connection between topological invariants and thermodynamic quantities.

KEY WORDS: Phase transitions; topology; configuration space; mean-field models.

[1] Istituto Nazionale per la Fisica della Materia (INFM), Unità di Ricerca di Firenze, via G. Sansone 1, I-50019 Sesto Fiorentino (FI), Italy; e-mail: casetti@fi.infn.it

[2] Istituto Nazionale di Astrofisica, Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, I-50125 Firenze, Italy; e-mail: pettini@arcetri.astro.it. Also at: INFM, UdR Firenze, and INFN, Sezione di Firenze, via G. Sansone 1, I-50019 Sesto Fiorentino (FI), Italy.

[3] The Rockefeller University, Box 28, 1230 York Avenue, New York, New York 10021-6399; e-mail: egdc@rockefeller.edu

1. INTRODUCTION

One can wonder whether the current mathematical description of thermodynamic phase transitions (based on the loss of analyticity of thermodynamic observables[1–3]) is the ultimate possible one, or whether a reduction to a deeper mathematical level is possible.

Besides a purely theoretical motivation, there are other reasons for thinking of such a possibility. Among the others, we mention the growing experimental evidence that phase transitions occur in very small N systems, like nuclear clusters as well as atomic and molecular clusters, in nano and mesoscopic systems, in polymers and proteins, in very small drops of quantum fluids (BEC, superfluids and superconductors).

Moreover, new mathematical characterizations of thermodynamic phase transitions could well be of interest for the treatment of other important topics in statistical physics, as is the case of amorphous and disordered systems (like glasses and spin-glasses), or to incorporate also first-order phase transitions. A different attempt than is discussed here has been made in macroscopic parameter space instead of in microscopic phase space in ref. 4.

In a number of recent papers[5–10] a proposal has been put forward for a new mathematical approach to the study of phase transitions. This applies to physical systems described by continuous variables—q_i and p_i, $i = 1,\dots, N$—entering a standard Hamiltonian

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

where $V(q_1,\dots, q_N)$ is the potential energy. The main issue of this new approach is a *Topological Hypothesis* (TH). The content of the TH is that at their deepest level phase transitions of a system are due to a change of the topology of suitable submanifolds in its configuration space. More precisely, once the microscopic interaction potential $V(q_1,\dots, q_N)$ is given, the configuration space of the system is automatically foliated into the family $\{\Sigma_v\}_{v\in\mathbb{R}}$ of equipotential hypersurfaces independently of any statistical measure we may wish to use. Now, from standard statistical mechanical arguments we know that the larger the number N of particles, the closer to some Σ_v are the microstates which significantly contribute to the statistical averages of thermodynamic observables. At large N, and at any given value of the inverse temperature β, the effective support of the canonical measure is narrowed very closely to a single hypersurface $\Sigma_v \equiv \{q \in \mathbb{R}^N \mid V(q) = v\} \subset \mathbb{R}^N$, with v a suitable function of β.

Now, the TH consists in assuming that some suitable change of the topology of the $\{\Sigma_v\}$, or equivalently, at large N, of the submanifolds

$M_v = \{q \in \mathbb{R}^N \mid V(q) \leqslant v\}$ (the manifolds Σ_v are the boundaries of the M_v, i.e., $\Sigma_v = \partial M_v$), occurring at some $v_c = v_c(\beta_c)$ (or $v_c = v_c(E_c)$), is the deep origin of the singular behavior of thermodynamic observables at a phase transition; (by change of topology we mean that $\{\Sigma_v\}_{v<v_c}$ are *not diffeomorphic*[4] to the $\{\Sigma_v\}_{v>v_c}$, or equivalently that $\{M_v\}_{v<v_c}$ are *not diffeomorphic* to the $\{M_v\}_{v>v_c}$). In the following of the paper we shall consider the topology changes of the M_v, because these are naturally investigated using Morse theory.

The present paper contributes to this new approach to phase transitions with a crucial step forward. This consists of an *exact analytic* treatment of the topology changes in the configuration space of the mean-field XY model and of their relation to the thermodynamic phase transition, reported in Section 2. In Section 3 we present an analogous treatment of a closely related model, the one-dimensional XY model with nearest-neighbors interactions, which does not have any thermodynamic phase transition, and we compare the results with those obtained for the mean-field case. In Section 4 we present and discuss a geometric model built in terms of two-dimensional surfaces which should help the intuition in understanding some of the aspects of the much more complex topology changes in N-dimensional configuration spaces. Section 5 is devoted to some final remarks and to the discussion of possible future developments. The paper is completed by Appendix A which is devoted to the proof of some crucial estimates used in the main text.

2. THE MEAN-FIELD *XY* MODEL

In this section we give a complete analytical characterization of the topological changes in the configuration space of a model with long-range interactions, the mean-field XY model, including the one related to the phase transition. This is, to our knowledge, the first complete analytical characterization of a topological change in configuration space related to a thermodynamic phase transition: a short account of this result has already been given in ref. 15. For a family of submanifolds of the configuration space defined by the potential energy, we are able—for the first time for a model of physical relevance—to determine completely, in a constructive way, the topology and to give analytical estimates of the Betti numbers, i.e., of fundamental topological invariants.[5] This allows us to compute

[4] A diffeomorphism is a smooth map between two differentiable manifolds which is invertible together with its derivatives.

[5] The Betti numbers b_k of a differentiable manifold M are the dimensions of the de Rham's cohomology vector spaces $\mathbb{H}^k(M; \mathbb{R})$, that is the vector spaces of closed differential k-forms modulo the exact forms of the same order. These are diffeomorphism invariants.

exactly a topological invariant: the Euler characteristic, which can be defined as a combination of the Betti numbers.(11)

The mean-field XY model(16) is defined by a Hamiltonian of the class (1) where the potential energy function is

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

Here $\varphi_i\in[0,2\pi]$ is the rotation angle of the i-th rotator and h is an external field. Defining at each site i a classical spin vector $\mathbf{s}_i=(\cos\varphi_i,\sin\varphi_i)$ the model describes a planar (XY) Heisenberg system with interactions of equal strength among all the spins. We consider only the ferromagnetic case $J>0$; for the sake of simplicity, we set $J=1$. The equilibrium statistical mechanics of this system is exactly described, in the thermodynamic limit, by mean-field theory. In the limit $h\to 0$, the system has a continuous phase transition, with classical critical exponents, at $T_c=1/2$, or $\varepsilon_c=3/4$, where $\varepsilon=E/N$ is the energy per particle.(16)

Defining the magnetization vector $\mathbf{m}$ as $\mathbf{m}=(m_x,m_y)$, where

$$m_x=\frac{1}{N}\sum_{i=1}^{N}\cos\varphi_i, \tag{3}$$

$$m_y=\frac{1}{N}\sum_{i=1}^{N}\sin\varphi_i, \tag{4}$$

the potential energy V can be written as a function of $\mathbf{m}$ as follows:

$$V(\varphi)=V(m_x,m_y)=\frac{N}{2}(1-m_x^2-m_y^2)-hN\,m_x. \tag{5}$$

The range of values of the potential energy per particle, $\mathscr{V}=V/N$, is then

$$-h\leqslant\mathscr{V}\leqslant\frac{1}{2}+\frac{h^2}{2}. \tag{6}$$

The configuration space M of the model is an N-dimensional torus, being parametrized by N angles. We want to investigate the topology of the following family of submanifolds of M,

$$M_v=\mathscr{V}^{-1}(-\infty,v]=\{\varphi\in M:\mathscr{V}(\varphi)\leqslant v\}, \tag{7}$$

i.e., each M_v is the set $\{\varphi_i\}_{i=1}^{N}$ such that the potential energy per particle does not exceed a given value v: this is the same as the $M_v=M_{E-K}$ defined above (v has been rescaled by $\frac{1}{N}$ because we choose $\mathscr{V}=V/N$ as a Morse function in order to make the comparison of systems with different N easier). As v is increased from $-\infty$ to $+\infty$, this family covers successively the whole manifold M ($M_v \equiv \emptyset$ when $v < -h$) .

According to Morse theory,[(12)] topology changes of M_v can occur only in correspondence with critical points of $\mathscr{V}$, i.e., those points where the differential of $\mathscr{V}$ vanishes. This immediately implies that no topology changes can occur 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. Moreover, if $\mathscr{V}$ is a Morse function (i.e., it has only non-degenerate critical points) then topology changes of M_v are actually in one-to-one correspondence with critical points of $\mathscr{V}$, and they can be characterized completely. At any critical level of $\mathscr{V}$ the topology of M_v changes in a way completely determined by the local properties of the Morse function: a k-handle $H^{(k)}$ is attached,[6] [(12)] where k is the *index* of the critical point, i.e., the number of negative eigenvalues of the Hessian matrix of $\mathscr{V}$ at this point. Notice that if there are $m > 1$ critical points on the same critical level, with indices $k_1, \ldots, k_m$, then the topology change is made by attaching m disjoint handles $H^{(k_1)}, \ldots, H^{(k_m)}$. This way, by increasing v, the topology of 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, defined by

$$\chi(M_v) = \sum_{k=0}^{N} (-1)^k \, \mu_k(M_v), \tag{8}$$

where the *Morse number* μ_k is the number of critical points of $\mathscr{V}$ which have index k.[(12)] The Euler characteristic χ is a *topological invariant* (i.e., it is not affected by a diffeomorphic deformation of M_v): any change in $\chi(M_v)$ implies a topology change in the M_v. It will turn out that as long as $h > 0$, $\mathscr{V}$ is indeed a Morse function at least in the interval $-h \leqslant v < 1/2 + h^2/2$, while the maximum value $v = 1/2 + h^2/2$ may be pathological in that it may correspond to a critical level with degenerate critical points. However, as we shall show in the following, we shall be able to extend our analysis also to this last critical level.

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

$$\frac{\partial \mathscr{V}(\varphi)}{\partial \varphi_i} = 0\,, \qquad i = 1, \ldots, N, \tag{9}$$

[6] A k-handle $H^{(k)}$ in n dimensions ($0 \leqslant k \leqslant n$) is the product of two disks, one k-dimensional, D^k, and one $(n-k)$-dimensional, $D^{(n-k)}$: $H^{(k)} = D^k \times D^{(n-k)}$.

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

$$H_{ij}=\frac{\partial^2\mathscr{V}}{\partial\varphi_i\partial\varphi_j}\qquad i,j=1,\ldots,N. \tag{10}$$

Taking advantage of Eq. (5), we can rewrite the Eq. (9) as

$$(m_x+h)\sin\varphi_i-m_y\cos\varphi_i=0,\qquad i=1,\ldots,N. \tag{11}$$

As long as (m_x+h) and m_y are not simultaneously zero (the violation of this condition is possible only on the level $v=1/2+h^2/2$), the solutions of Eq. (11) are all configurations in which the angles are either 0 or π. In particular, the configuration

$$\varphi_i=0\qquad\forall\, i \tag{12}$$

is the absolute minimum of $\mathscr{V}$, while all the other configurations correspond to a value of v which depends only on the number of angles which are equal to π. If we denote with n_π this number, we have that the N critical values are:

$$v(n_\pi)=\frac{1}{2}\left[1-\frac{1}{N^2}(N-2n_\pi)^2\right]-\frac{h}{N}(N-2n_\pi). \tag{13}$$

Inverting this relation yields n_π as a function of the level value v:

$$n_\pi(v)=\mathrm{int}\left[\frac{1+h}{2}N\pm\frac{N}{2}\sqrt{h^2-2\left(v-\frac{1}{2}\right)}\right], \tag{14}$$

where int$[a]$ stands for the integer part of a. We can also compute the number $C(n_\pi)$ of critical points having a given n_π, which is the number of distinct binary strings of length N having n_π occurrences of one of the symbols, which is given by the binomial coefficient

$$C(n_\pi)=\binom{N}{n_\pi}=\frac{N!}{n_\pi!\,(N-n_\pi)!}. \tag{15}$$

We have thus shown that as v changes from its minimum $-h$ (corresponding to $n_\pi=0$) to $\frac{1}{2}$ (corresponding to $n_\pi=\frac{N}{2}$) the manifolds M_v undergo a sequence of topology changes at the N critical values $v(n_\pi)$ given by

Eq. (13). We expect that there is another topology change located at the last (maximum) critical value,

$$v_c = \frac{1}{2} + \frac{h^2}{2}. \tag{16}$$

However, the above argument does not prove this, since the critical points of $\mathscr{V}$ corresponding to this critical level may be degenerate. This, because the solutions of the two equations in N variables $m_x = m_y = 0$ need not to be isolated, so that then on this level, $\mathscr{V}$ would not be a proper Morse function. Then a critical value v_c is still a necessary condition for the existence of a topology change, but it is no longer sufficient.[13] However, as already argued in refs. 7 and 9, it is just this topology change occurring at v_c given in Eq. (16), which is related to the thermodynamic phase transition of the mean-field XY model. For, the temperature T, the energy per particle ε and the average potential energy per particle $u = \langle \mathscr{V} \rangle$ obey, in the thermodynamic limit, the equation

$$2\varepsilon = T + 2u(T); \tag{17}$$

substituting in this equation the values of the critical energy per particle and of the critical temperature we get

$$u_c = u(T_c) = 1/2. \tag{18}$$

as $h \to 0$, $v_c \to \frac{1}{2}$, so that $v_c = u_c$. Thus a topology change in the family of manifolds M_v occurring at this v_c, where v_c is *independent* of N, is connected with the phase transition in the limit $N \to \infty$, and $h \to 0$, when indeed thermodynamic phase transitions are usually defined, at least in the canonical ensemble.

We still have to prove that a topology change at v_c actually exists. To carry out this proof, we will use Morse theory to characterize completely all the other topology changes, occurring at $v < v_c$: this, together with the knowledge that at $v > v_c$ the manifold M_v must be an N-torus, will allow us not only to prove that a topology change at v_c must actually occur, but also to understand in which way it is different from the other topology changes, i.e., those occurring at $0 \leqslant v < v_c$. Morse theory allows a complete characterization of the topology changes occurring in the M_v's if the *indices* of the critical points of $\mathscr{V}$ are known. In order to determine the indices of the critical points (that is the number of negative eigenvalues of the Hessian of $\mathscr{V}$ at the critical point) we proceed as follows. Since the diagonal elements of the Hessian are

$$H_{ii} = d_i = \frac{1}{N}\left[(m_x + h)\cos\varphi_i + m_y \sin\varphi_i\right] - \frac{1}{N^2}, \tag{19}$$

and the off-diagonal elements are

$$H_{ij} = -\frac{1}{N^2}(\sin\varphi_i \sin\varphi_j + \cos\varphi_i \cos\varphi_j), \tag{20}$$

one can write the Hessian as the sum of a diagonal matrix D whose nonzero elements are

$$\delta_i = \frac{1}{N}\left[(m_x + h)\cos\varphi_i + m_y \sin\varphi_i\right], \qquad i = 1,\dots, N, \tag{21}$$

and of a matrix B whose elements are just the H_{ij} given in Eq. (20), also for $i = j$ (the diagonal elements being $-1/N^2$). Since the ratio between the elements of B and those of D is $\mathcal{O}(1/N)$, one would expect at first sight that only the diagonal elements survive when $N \gg 1$, so that the Hessian approaches a diagonal matrix equal to D. However, this is not, in principle, necessarily true: one cannot immediately say that at large N the eigenvalues of the Hessian are the δ's given in Eq. (21) plus a correction vanishing as $N \to \infty$, because the number of elements of B is N^2, so that the contribution of the matrix B to the eigenvalues of the Hessian does *not*, in general, vanish at large N. That nevertheless the argument for this crucial point is correct in this special case is shown in Appendix A, and is due to the particular structure of the matrix B. The latter is of rank one, and one can prove then that at the critical points of $\mathscr{V}$ the number of negative eigenvalues of H equals the number of negative diagonal elements $\delta \pm 1$, so that as $N \gg 1$ we can conveniently approximate the index of the critical points with the number of negative δ's at x,

$$\text{index}(x) \simeq \#(\delta_i < 0). \tag{22}$$

At a given critical point, with given n_π, where the x-component of the magnetization vector is

$$m_x = 1 - \frac{2n_\pi}{N}, \tag{23}$$

so that $m_x > 0$ (resp. < 0) if $n_\pi \leqslant \frac{N}{2}$ (resp. $> \frac{N}{2}$), the eigenvalues of D are

$$\delta_i = m_x + h \qquad i = 1, \ldots, N - n_\pi; \tag{24a}$$

$$\delta_i = -(m_x + h) \qquad i = N - n_\pi + 1, \ldots, N. \tag{24b}$$

Then, if the external field h is sufficiently small,

$$\begin{aligned} (m_x + h) > 0 \qquad &\text{if} \quad n_\pi \leqslant \frac{N}{2}, \\ (m_x + h) < 0 \qquad &\text{if} \quad n_\pi > \frac{N}{2}, \end{aligned} \tag{25}$$

so that, denoting with index(n_π) the index of a critical point with n_π angles equal to π, we can write

$$\mathrm{index}(n_\pi) = n_\pi \qquad \text{if} \quad n_\pi \leqslant \frac{N}{2}, \tag{26a}$$

$$\mathrm{index}(n_\pi) = N - n_\pi \qquad \text{if} \quad n_\pi > \frac{N}{2}. \tag{26b}$$

From these equations combined with Eq. (15) one can obtain for the Morse numbers μ_k, i.e., for the number of critical points of index k, as a function of the level v, as long as $-h \leqslant v < 1/2 + h^2/2$ (i.e., excluding the limiting value $v = 1/2 + h^2/2$) the following expression:

$$\mu_k(v) = \binom{N}{k} [1 - \Theta(k - n^{(-)}(v)) + \Theta(N - k - n^{(+)}(v))], \tag{27}$$

where $\Theta(x)$ is the Heaviside theta function and $n^{(\pm)}(v)$ are the limits of the allowed n_π's for a given value of v, i.e., from Eq. (14),

$$n^{(\pm)}(v) = \frac{N}{2}\left[1 + h \pm \sqrt{h^2 - 2\left(v - \frac{1}{2}\right)}\right]. \tag{28}$$

We note that $0 \leqslant n_\pi^{(-)} \leqslant \frac{N}{2}$ and $\frac{N}{2} + 1 \leqslant n_\pi^{(+)} \leqslant N$, so that Eq. (27) implies

$$\mu_k(v) = 0 \qquad \forall\, k > \frac{N}{2}, \tag{29}$$

i.e., no critical points with index larger than $N/2$ exist as long as $v < v_c = 1/2 + h^2/2$. This is the crucial observation to prove that a topology change *must* occur at v_c. For, as the Betti numbers of a manifold are positive (or zero) numbers, using the Morse inequalities, which state that the Morse numbers are upper bounds of the Betti numbers,[13] i.e.

$$b_k \leqslant \mu_k \qquad \text{for} \quad k=0,\dots, N, \tag{30}$$

we can immediately conclude that as long as $v < v_c = 1/2 + h^2/2$

$$b_k(M_v) = 0 \qquad \forall\, k > \frac{N}{2}. \tag{31}$$

Thus, as $\frac{1}{2} \leqslant v < \frac{1}{2} + \frac{h^2}{2}$ the manifold is only "half" an N-torus, and since we know that for $v > \frac{1}{2} + \frac{h^2}{2}$, M_v *is* a (full) N-torus, whose Betti numbers are

$$b_k(\mathbb{T}^N) = \binom{N}{k} \qquad k = 0, 1,\dots, N, \tag{32}$$

we conclude that at $v = v_c = \frac{1}{2} + \frac{h^2}{2}$ a topology change *must* occur, which involves the attaching of $\binom{N}{k}$ different k-handles for each k ranging from $\frac{N}{2}+1$ to N, i.e., a change of $\mathcal{O}(N)$ of the number of Betti numbers.

Let us remark that such a topology change not only exists: it is surely a "big" topology change, for all of a sudden, "half" an N-torus becomes a full N-torus, via the attaching for each different k (ranging from $N/2+1$ to N) of $\binom{N}{k}$ k-handles. More precisely, a number of Betti numbers which is $\mathcal{O}(N)$ changes, and changes by amounts which are of the same order as their maximum possible values. On the other hand, all the other topology changes correspond to the attaching of handles of the same type (index), in fact, as long as $v < v_c$, each critical level contains only critical points of the same index, and the index grows with v, i.e., if x_c and x'_c are critical points and $\mathscr{V}(x'_c) > \mathscr{V}(x_c)$, then $\mathrm{index}(x'_c) > \mathrm{index}(x_c)$. The potential energy per degree of freedom $\mathscr{V}$ is a *regular* Morse function (or a Morse–Smale function[13]) as long as $v < v_c$, but this is no longer true as $v \geqslant v_c$; actually, as we have already observed, $\mathscr{V}$ could even be no longer a Morse function at all, because the level v_c might contain degenerate critical points. Nevertheless, as we have shown, this does not prevent us from giving a complete analysis of the topology of the M_v's for *all* the values of v, since we can exploit our explicit knowledge of the topology of the M_v's for any $v > v_c$.

To illustrate what we have described so far, the Morse numbers μ_k are shown in Fig. 1 as a function of k for two values of v, $v = \frac{1}{4}$, i.e., an intermediate value between the minimum and the maximum of $\mathscr{V}$—shown in Fig. 1(a)—and $v = \frac{1}{2}$—shown in Fig. 1(b). We see that the μ_k with $0 \leqslant k \leqslant \frac{N}{2}$ grow regularly as v grows until $v_c = \frac{1+h^2}{2}$, while all the μ_k with $k > \frac{N}{2}$ remain

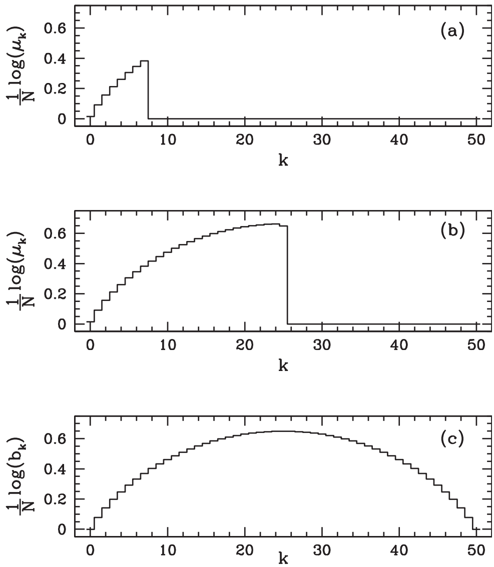

Fig. 1. Mean-field XY model. (a) Histogram of $\log(\mu_k(M_v))/N$ as a function of k for $v = 1/4$; (b) Histogram of $\log(\mu_k(M_v))/N$ as a function of k for $v = 1/2$. In both cases $N = 50$ and $h = 0.01$. (c) For comparison, histogram of $\log(b_k(\mathbb{T}^N))/N$ as a function of k for an N-torus $\mathbb{T}^N$, with $N = 50$, which is the lower bound of $\log(\mu_k(M_v))/N$ for any $v \geqslant v_c$.

zero, so that also the corresponding Betti numbers must vanish. But at v_c a dramatic event occurs, because for all the values of $v > v_c$ the Betti numbers b_k *must* be those of an N-torus, which are reported for comparison in Fig. 1(c). A sudden transition from the situation depicted in Fig. 1(b) to that of Fig. 1(c) occurs at v_c, i.e., $\frac{N}{2}$ Betti numbers simultaneoulsy become nonzero.

Now we are in a position to explain how these topological transitions can be described by topological invariants. The optimal situation would be the possibility of computing all the $N+1$ Betti numbers of the manifolds M_v as a function of v: unfortunately, we are only able to set an upper limit to them, using the Morse inequalities (30). Nevertheless, we can use Eqs. (8), (14), and (27) to compute the Euler characteristic of the manifolds M_v, since we only need the μ_k for that. It turns out then that χ jumps from positive to negative values, so that it is easier to look at $|\chi|$. In Fig. 2, $\log(|\chi|(M_v))/N$ is plotted as a function of v for various values of N ranging from 50 to 800. The "big" topology change occurring at the maximum value of $\mathscr{V}$, which corresponds in the thermodynamic limit to the phase transition, implies a discontinuous jump of $|\chi|$ from a big value to zero.

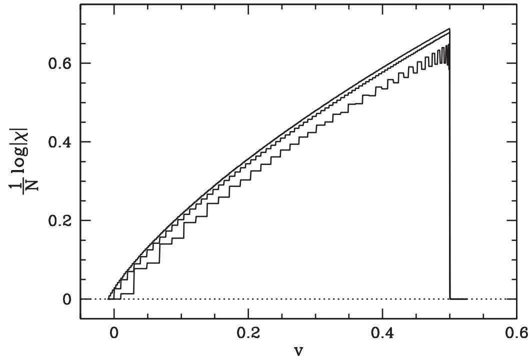

Fig. 2. Mean-field XY model. Plot of $\log(|\chi|(M_v))/N$ as a function of v. $N=50$, 200, 800 (from bottom to top) and $h=0.01$; $v_c=0.5+\mathcal{O}(h^2)$.

3. THE ONE-DIMENSIONAL *XY* MODEL

We consider now one example where there are topological changes very similar to the ones of the mean-field XY model but no phase transition occurs, i.e., the one-dimensional XY model with nearest-neighbor interactions, whose Hamiltonian is of the class (1) with interaction potential

$$V(\varphi)=\tfrac{1}{4}\sum_{i=1}^{N}\left[1-\cos(\varphi_{i+1}-\varphi_i)\right]-h\sum_{i=1}^{N}\cos\varphi_i. \tag{33}$$

In this case the configuration space M is still an N-torus, and using again the interaction energy per degree of freedom $\mathcal{V}=V/N$ as a Morse function, we can prove that also here there are many topological changes in the submanifolds M_v as v is varied from its minimum to its maximum value.

The critical points are again those where the φ_i' s are equal either to 0 or to π. However, at variance with the mean-field XY model, the critical values are now determined by the number of domain walls, n_d, i.e., the number of boundaries between connected regions on the chain where the angles are all equal ("islands" of π's and "islands" of 0's). The number of π's leads only to a correction $\mathcal{O}(h)$ to the critical value of v, which is given by

$$v(n_d;n_\pi)=\frac{n_d}{2N}+h\,n_\pi. \tag{34}$$

Since $n_d\in[0,N-1]$ (with free boundary conditions, $n_d=0,1,\ldots,N-1$, while with periodic boundary conditions n_d is still bounded by 0 and $N-1$, but can only be even), the critical values lie in the same interval as in the case of the mean-field XY model. But now the maximum critical value, instead of corresponding to a huge number of critical points, which rapidly grows with N, corresponds to *only two* configurations with $N-1$ domain walls, which are $\varphi_{2k}=0$, $\varphi_{2k+1}=\pi$, with $k=1,\dots,N/2$, and the reversed one.

The number of critical points with n_d domain walls is therefore (assuming free boundary conditions)

$$\mathcal{N}(n_d)=2\binom{N-1}{n_d}. \tag{35}$$

We can compute the index of the critical points also in this case (see Appendix A.2 for details). It turns out that

$$\text{index}(n_d)=n_d, \tag{36}$$

so that

$$\mu_k(n_d)=2\binom{N-1}{k}\Theta(n_d-k). \tag{37}$$

It is evident then that any topology change here corresponds to the attaching of handles of the same type. However, no "big" change like the one at v_c in the case of the mean-field model exists, although $\mathcal{V}$ is a Morse–Smale function on the whole manifold M. To illustrate this, we plot in Fig. 3 the values of the Morse indices μ_k as a function of k, as we have already done for the mean-field XY model in Fig. 1. Comparing Fig. 3 with Fig. 1, we see that while in the mean-field model there is a critical value where $\frac{N}{2}$ Betti numbers become simultaneously nonzero, i.e., there exists a topology change which corresponds to the simultaneous attaching of handles of $\frac{N}{2}$ different types, while here in the one-dimensional nearest-neighbor model nothing like that happens.

Also in this case, using Eqs. (35) and (36), we can compute the Euler characteristic of the submanifolds M_v:

$$\chi(M_v)=2\sum_{k=0}^{n_d(v)}(-1)^k\binom{N-1}{k}=2\,(-1)^{n_d(v)}\binom{N-2}{n_d(v)}, \tag{38}$$

where, due to Eq. (34),

$$n_d(v)=2Nv+\mathcal{O}(h). \tag{39}$$

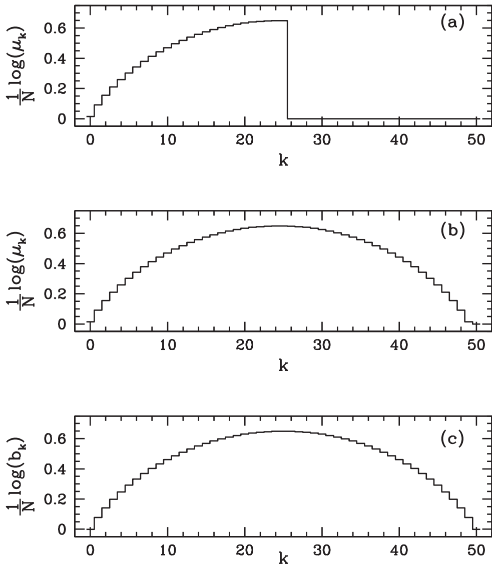

Fig. 3. The same as Fig. 1 for the one-dimensional XY model with nearest-neighbor interactions. (a) Histogram of $\log(\mu_k(M_v))/N$ as a function of k for $v = 1/4$; (b) Histogram of $\log(\mu_k(M_v))/N$ as a function of k for $v = 1/2$. In both cases $N =$ 50 and $h = 0.01$. (c) For comparison, histogram of $\log(b_k(\mathbb{T}^N))/N$ as a function of k for an N-torus $\mathbb{T}^N$, with $N = 50$.

The Euler characteristic for the one-dimensional nearest-neighbor case is shown in Fig. 4. Comparing this figure with Fig. 2, we see that there is here no jump in the Euler characteristic.

Before discussing the relevance that these results may have for the general problem of the relation between topology and phase transitions, it

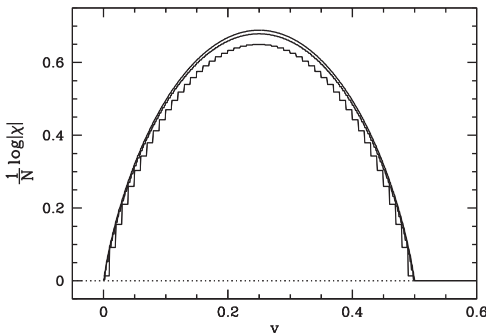

Fig. 4. Plot of $\log(|\chi|(M_v))/N$ for the one-dimensional XY model with nearest-neighbor interactions as a function of v. $N =$ 50, 200, 800 (from bottom to top).

is illustrative to consider two abstract simplified models of topological transitions that occurred in the two models we have considered so far.

4. TWO-DIMENSIONAL MODEL OF TOPOLOGY CHANGES

A two-dimensional model of the topological transition occurring in the configuration space of the physical models we have discussed, which could perhaps help the intuition, can be built as follows. Let us consider a two-dimensional torus $\mathbb{T}$, and place it on a plane: let $h_{\max}$ be the maximum height of the surface above the plane (see Fig. 5(a)). Then deform the torus (by means of a diffeomorphism) until the upper end of the hole is at height $h_{\max} - \varepsilon$, obtaining the surface M shown in Fig. 5(b). It is apparent that ε can be made as small as we want.

Let us now consider the height function $\mathscr{H}$ above the plane as a Morse function, so that the manifolds

$$\mathbb{T}_h = \mathscr{H}^{-1}(-\infty, h] = \{x \in \mathbb{T} : \mathscr{H}(x) \leqslant h\} \tag{40}$$

$$M_h = \mathscr{H}^{-1}(-\infty, h] = \{x \in M : \mathscr{H}(x) \leqslant h\} \tag{41}$$

are defined. As h varies from its minimum to its maximum values ($h = 0$ and $h = 3$, respectively, in Fig. 5), the manifolds $\mathbb{T}_h$ and M_h cover the whole torus; as long as h is lower than the top of the hole ($h = 2$ in Fig. 5), both $\mathbb{T}_h$ and M_h are "half-tori," but then the $\mathbb{T}_h$ become *gradually* a full torus, while the M_h jump abruptly from a half-torus to a full torus as h is changed by ε. Identifying the height function with the potential energy, the case of the $\mathbb{T}_h$ clearly reminds of the behavior of the one-dimensional XY model with no phase transition, while the case of the M_h seems close to

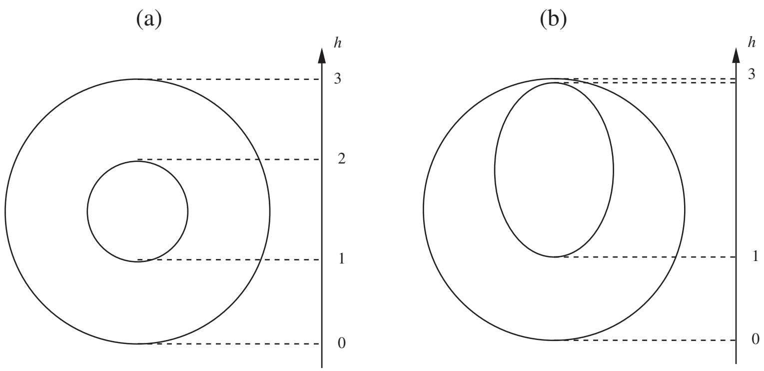

Fig. 5. (a) A torus $\mathbb{T}$ and its height function. Here $h_{\max} = 3$. (b) A deformation M of such a torus as explained in the text.

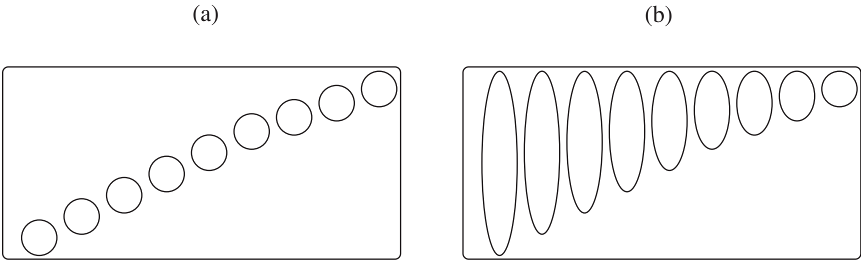

Fig. 6. (a) A surface of high genus (here $g=9$). (b) A deformation $M^{(g)}$ of such a surface as explained in the text.

what happens in the mean-field XY model, and the "jump" from the half-torus to the full torus is similar to the topology change which is connected to the phase transition.

The analogy with the mean-field models becomes even clearer if, instead of a torus, we consider a compact surface of genus[7] $g \gg 1$, i.e., with many holes, and deform the surface with a diffeomorphism until the upper end of all the holes is at height $h_{\max}-\varepsilon$, as shown in Fig. 6. Again, ε can be made as small as we want. Let us denote by $M^{(g)}$ the deformed surface.

The Betti numbers of the surface $M^{(g)}$ are[22]

$$b_0 = b_2 = 1\,, \qquad b_1 = 2g, \tag{42}$$

and the Euler characteristic is

$$\chi(M^{(g)}) = \chi(M^{(g)}) = 2-2g, \tag{43}$$

i.e., a big negative number. Let us now consider, as in the previous case of the torus, the height function $\mathscr{H}$ above the plane as a Morse function. The manifolds

$$M_h^{(g)} = \mathscr{H}^{-1}(-\infty, h] = \{x \in M^{(g)} : \mathscr{H}(x) \leqslant h\} \tag{44}$$

will be topologically very different from the whole $M^{(g)}$ as long as $h < h_{\max}-\varepsilon$ but sufficiently large that all the critical levels corresponding to the bottoms of all the holes have already been crossed: in fact, their Betti numbers will be

$$b_0(M_h^{(g)}) = 1, \qquad b_1(M_h^{(g)}) = g, \qquad b_2(M_h^{(g)}) = 0, \tag{45}$$

[7] The *genus* g is the number of handles of a two-dimensional surface.

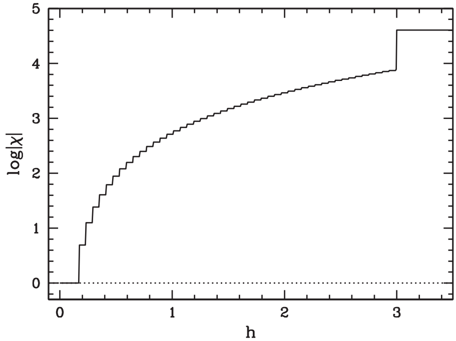

Fig. 7. Plot of the logarithm of the absolute value of the Euler characteristic of the submanifolds of given height of a surface $M^{(g)}$ like the one depicted in Fig. 6(b), with $g = 50$ and $h_{\max} = 3$, as a function of the height h. The small jumps are the topology transitions corresponding to the crossing of the bottoms of the holes: the last big jump is the one occurring at $h_{\max}$, when $\varepsilon \to 0$.

and the Euler characteristic will be

$$\chi(M_h^{(g)}) = 1 - g. \tag{46}$$

Then, by changing the value of the height by an amount ε as small as one wants, one changes the Betti number b_1 from g to $2g$, the b_2 from 0 to 1 and χ from $1-g$ to $2-2g$. This is a topological change which involves a change of $\mathcal{O}(d)$ Betti numbers (d is the dimension of the manifold); moreover, the size of the change is of the order of the value of the Betti numbers. This topology change involves also a change of the Euler characteristic χ which is again of the same order as its value. Identifying again the height function with the potential energy, we see that this is just what happens in the case of the M_v of the mean-field XY model, although there the dimension of the manifolds is N and very large, while in this low-dimensional analogy it is only $d = 2$. The behavior of $|\chi(M_h^{(g)})|$ as a function of h is plotted in Fig. 7. We see that the behavior of $|\chi|$ is indeed very similar to the case of the mean-field XY model, the only big difference being that in the latter $|\chi|$ jumps to zero while here it jumps to a nonzero value. However this difference is due to the fact that the Euler characteristic of a torus is zero while that of a surface of genus g is $2-2g$.

5. CONCLUDING REMARKS AND OPEN QUESTIONS

We conclude with some comments and remarks, and with a discussion of the open problems and of the future perspectives opened by the results we have presented.

5.1. Topology and Thermodynamic Functions

The results we have reported in the present paper concerning the mean-field and the one-dimensional XY models, together with a theorem[14] which states the necessity of topology changes in the M_v's for the existence of phase transitions (at least for a certain class of short-range interactions), lend strong support to the TH. However, one could wonder whether a direct relation between topology and thermodynamic quantities, like entropy or temperature, exists.

A result—although approximate—which shows that there could be an explicit contribution of topological quantities to the temperature was indeed found in a previous paper:[10] it relates the inverse temperature $\beta = \frac{1}{T}$ to the Betti numbers b_i of the constant-energy hypersurface in phase space, Σ_E. We stress the fact that such a relation—Eq. (43) in ref. 10—does not allow to express β in terms of topological invariants alone, because also other contributions, of a non-topological nature, exist: nonetheless a topological contribution expressed as a function of the Betti numbers of Σ_E is explicitly present. A similar relation can be obtained also for the entropy: the derivation only involves a slight modification of the reasoning of Sec. V of ref. 10. Without entering into technical details, we simply observe that, under the same approximations as made in ref. 10, the "topological contribution" $\tau(E)$ to the entropy per degree of freedom $s = \frac{S}{N}$ can be written, up to constant terms, as

$$\tau(E) \simeq \frac{1}{2N-1} \log \sum_{i=0}^{2N-1} b_i(\Sigma_E), \tag{47}$$

an expression identical to the corresponding expression for β in ref. 10, apart from the presence of a logarithm here. We remark that, as in the case of β, there are also other contributions, of a non-topological nature, to the entropy. However, it is interesting to look at this topological τ-contribution alone to see whether it carries the relevant information about the way the topological transition of the energy hypersurface in phase space triggers the phase transition, i.e., the nonanalyticity of the thermodynamic quantities. Therefore we can try to compute τ for the models studied in the present paper.

First of all, we have to express $\tau(E)$ in terms of the topological invariants of the manifolds M_v instead of in terms of the Betti numbers of the energy hypersurfaces Σ_E [Eq. (47)]. To do that, we resort to the fact that—at large N and for systems with standard kinetic energy K—the volume measure of Σ_E concentrates on[8] $\mathbb{S}^{N-1}_{\langle 2K\rangle^{1/2}} \times M_{\langle V\rangle}$, so that Σ_E can be

[8] $\mathbb{S}^{N-1}_{\langle 2K\rangle^{1/2}}$ is an $N-1$-dimensional hypersphere defined by the kinetic energy term $\sum p_i^2 = 2\langle K\rangle$. We have $E = \langle K\rangle + \delta K + \langle V\rangle + \delta V$, and $\delta K/\langle K\rangle, \delta V/\langle V\rangle = \mathcal{O}(1/\sqrt{N})$.

approximated by this product manifold. Using then the Kunneth formula[11] for the Betti numbers of a product manifold $A \times B$, i.e.,

$$b_i(A \times B) = \sum_{j+k=i} b_j(A)\, b_k(B) \tag{48}$$

which, when applied to $\mathbb{S}^{N-1}_{\langle 2K \rangle^{1/2}} \times M_{\langle V \rangle}$, gives $b_i(\Sigma_E) = 2b_i(M_v)$ for $i = 1,\dots, N-1$, and $b_j(\Sigma_E) = b_j(M_v)$ for $j = 0$, N, since all the Betti numbers of a hypersphere vanish except b_0 and b_N which are equal to 1. This allows us to write

$$\tau(v) \simeq \frac{1}{2N} \log \left[b_0(M_v) + 2 \sum_{i=1}^{N-1} b_i(M_v) + b_N(M_v) \right], \tag{49}$$

where we have also replaced $2N-1$ with $2N$ because we assume that N is large. Since we cannot compute the Betti numbers exactly, we cannot evaluate this expression; nonetheless, we can estimate it by using the Morse numbers as approximations of the Betti numbers, i.e., by putting

$$b_i(M_v) \simeq \mu_i(M_v), \qquad i = 0,\dots, N. \tag{50}$$

In general, with the exception of perfect Morse functions (i.e., those for which $b_i = \mu_i$), the Morse numbers are only upper bounds of the Betti numbers. However, looking at Figs. 1(b)–(c) (for the mean-field XY model) and 3(b)–(c) (for the one-dimensional XY model), we can observe that the nonvanishing Morse numbers of the manifolds M_v for values of v very close to $v_{\max}$ are very close to the Betti numbers of the M_v's for $v = v_{\max}$ (which are N-tori), and this suggests that for the models studied in the present paper the Morse numbers μ_i could well be good approximations to the Betti numbers b_i.

We can then compute the quantity

$$\tilde{\tau}(v) = \frac{1}{2N} \log \left[\mu_0(M_v) + 2 \sum_{i=1}^{N-1} \mu_i(M_v) + \mu_N(M_v) \right], \tag{51}$$

for the two models studied in the paper. We note that

$$\sum_{i=0}^{N} \mu_i(M_v) = N_c(M_v), \tag{52}$$

where $N_c(M_v)$ is the total number of critical points of the function $\mathscr{V}$ in the manifold M_v. Therefore, when N gets large, and if μ_0 and μ_N are not much

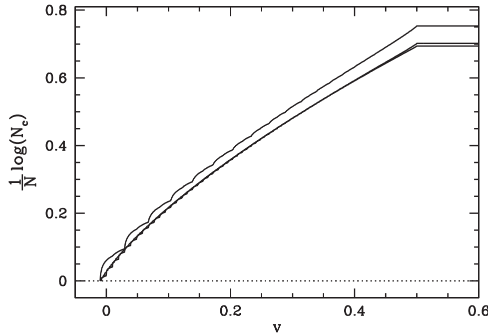

Fig. 8. Mean-field XY model. Plot of $\log(N_c)/N$ as a function of v. $N = 50$, 200, 800 (from top to bottom) and $h = 0.01$; $v_c = 0.5 + \mathcal{O}(h^2)$.

larger than the other Betti numbers (which is true in our case, see Fig. 1), we can write approximately

$$\tilde{\tau}(v) \simeq \frac{1}{N} \log N_c(v), \tag{53}$$

apart from an additive constant. The behavior of this quantity is plotted as a function of v in Fig. 8 for the mean-field XY model and in Fig. 9 for the one-dimensional XY model. First, we note that in both cases the "topological contribution" $\tilde{\tau}$ to the entropy behaves qualitatively as expected for the configurational entropy, i.e., it grows monotonically up to the maximum value of v, after which it remains constant. Moreover, we see that, in the case of the mean-field model (Fig. 8), the topology change at v_c related to the phase transition corresponds to a discontinuity in the slope of $\tilde{\tau}(v)$, which thus seems to be both the precursor and the source of the

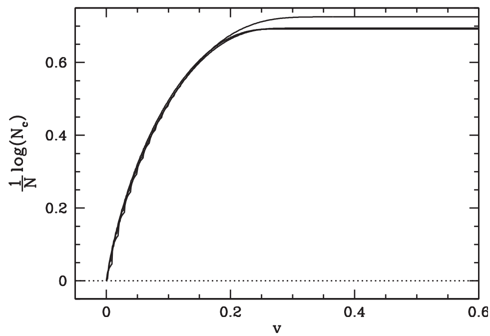

Fig. 9. One-dimensional XY model with nearest-neighbor interactions. Plot of $\log(N_c)/N$ as a function of v. $N = 50$, 200, 800 (from top to bottom) and $h = 0.01$.

nonanalyticity of the entropy at the phase transition point as $N \to \infty$. In the case of the one-dimensional XY model, where no phase transition is present, unlike the mean-field case, the curve is smooth for any v, consistent with the fact that also the entropy of the system is smooth.

Therefore the contribution of the Betti numbers alone to the thermodynamic quantity s appears to yield the phase transition point correctly; an indication again of the topological mechanism of the phase transition.

We emphasize that the discontinuity in Fig. 2 at $v = v_c$ corresponds to that of Fig. 8 at the same value of v. Even more, the many small jumps in the Euler characteristic occurring in Fig. 2, and corresponding to the topological changes which occur at $v < v_c$, are smoothed out in Fig. 8 where the topological contribution to the entropy, $\tilde{\tau}$, is reported. This is due to the fact that while the Euler characteristic is the alternating sum of the Morse numbers μ_i, the τ is the sum of them: this is a further indication that to yield a phase transition, i.e., a discontinuity in a derivative of s, a "strong" topology change would be needed, such as to affect the variation of the sum of all the Betti numbers as a function of v.

However, to what extent these results are of general validity remains an interesting open question.

5.2. When Does a Topology Change Entail a Phase Transition?

Another fundamental point which still remains open in the topological approach to phase transitions is the question of which are the *sufficient* conditions for the topology changes of the manifolds M_v to entail a phase transition. Topology changes appear to be rather common, and most of them are *not* connected to phase transitions.

In our previous papers, clear evidence—albeit only numeric—was found that phase transitions would correspond to very significant transitions in the way the topology changes[8] as a function of v. Moreover, in Section 5.1 we have discussed a possible mechanism through which a topological change could trigger a change in the properties of thermodynamic functions, resulting in a phase transition.

On the basis of our results obtained before and here, we put forward the conjecture that what we have observed in the case of XY models may well have general validity: a topology change in the submanifolds M_v might entail a phase transition if it involves the simultaneous attachment of handles of $\mathcal{O}(N)$ different types on the same critical level. However, we must be aware that this could well be specific to the class of models studied here: to what extent this conjecture might have general validity remains an open question.

5.3. The Role of the External Field *h*

Studying the topology changes in the configuration space of XY models, mean-field as well as one-dimensional, we have considered the presence of an external field $h \neq 0$ which explicitly breaks the $O(2)$-invariance of the potential energy, and then, discussing the connection with phase transitions, we have considered the case in which h tends to zero. We did that for the sake of simplicity, for, if we set $h = 0$ from the outset, the potential energy per degree of freedom $\mathscr{V}$ is *not*, rigorously speaking, a Morse function, because its $O(2)$-invariance entails the presence of a zero eigenvalue in its Hessian. When $h = 0$, the critical points of $\mathscr{V}$ are *not* isolated, but form one-dimensional manifolds (topologically equivalent to circles) which are left unchanged by the action of the $O(2)$ continuous symmetry group so that the critical points become in this case critical manifolds. However, in the case of the mean-field XY model, as far as the presence and the nature of topology changes are concerned, studying the case with $h = 0$ from the outset we find *exactly* the same behavior as in the case we have discussed in this paper, i.e., as long as $v < v_c$ only handles of the same type are attached, while at $v = v_c$ handles of $N/2$ different types are attached, the only difference between the two cases being that when $h = 0$ the handles are not attached at isolated points, but rather to the entire critical manifold.[12, 13] However, putting $h = 0$ from the beginning makes the computation of the Euler characteristic $\chi(M_v)$ via the Morse numbers much more difficult, because now one has to take into account the contributions to χ coming from the Betti numbers of the critical manifolds (see ref. 20 for the details).

In the case of the one-dimensional nearest-neighbor XY model, where no phase transition is present, the use of $h = 0$ from the outset implies a further complication, i.e., that the critical points consist not only of the configurations made of 0's and π's, but also of spin waves, that is configurations

$$\varphi_j = \varphi_0 \, e^{ikj}, \tag{54}$$

with wavenumbers k depending on boundary conditions.

For all these reasons we preferred to force the potential energy to be a Morse function via the explicit breaking of the $O(2)$ symmetry using an external field $h \neq 0$. Incidentally, we notice that in the mean-field XY model, as long as $h \neq 0$, the topology changes which do not correspond to any phase transition (i.e, those occurring at $v < v_c$) occur at a number of values of v which grows with N, and these values become closer and closer as N grows, eventually filling the whole interval $[0, \frac{1}{2}]$ as $N \to \infty$. To the contrary, the value v_c, which corresponds to the "big" topology change connected to the phase transition, remains separated from the others by an amount $\mathcal{O}(h^2)$ also in the thermodynamic limit, and tends to $\frac{1}{2}$ only when $h \to 0$. This is reminiscent of a similar fact occurring in statistical mechanics, where one observes a spontaneous symmetry breaking, signalled, e.g., by the onset of a finite magnetization even at zero external field, if one assumes the presence of an external field and then lets it tend to zero only after the thermodynamic limit is taken.

5.4. Transitional Phenomena in Finite Systems and Other Future Developments

(a) If it would be possible to establish a one-to-one correspondence between a particular class of topology changes in configuration space and the usual thermodynamic phase transitions defined in the thermodynamic limit, then, as a by-product, one would have available also a natural definition of phase transitions for *finite* systems. In fact, the topology changes are defined at any N, so that one would call "phase transitions at finite N" those topology changes in configuration space which become phase transitions in the usual, statistical-mechanical sense at infinite N. This would be an interesting consequence of the present topological approach to phase transitions, since it would circumvent the basic problem of any clear definition of phase transitions at finite N, by showing that all phase transitions have their basic origin in a topological change which may occur also at finite N, but entail true mathematical singularities in the thermodynamic functions only at infinite N.

(b) Finite systems do not seem to be the only active field of statistical physics where the topological approach might prove useful. Another promising field of application is that of glasses or, in general, of disordered systems. It is now quite clear that many of the puzzling properties of glasses are encoded in their "energy landscape",[18] i.e., in the structure of valleys and saddles of the potential energy function: but this is directly connected to the structure of the submanifolds M_v and Σ_v of configuration space, and in fact topological concepts start to emerge in some recent papers on glasses.[19]

(c) Finally, we notice that at present only systems undergoing second-order phase transitions have been studied via the topological approach: a natural question which arises is then if also first-order transitions can be explained topologically. Work is in progress in this direction, and some preliminary results indicate that also discontinuous phase transitions can be connected to topology changes of the submanifolds M_v, and that a signature of them can be found in their Euler characteristic.

APPENDIX A. ESTIMATE OF THE INDEX OF THE CRITICAL POINTS

In this Appendix we want to discuss some details related to the estimates of the indices of the critical points we have used in Section 2 and Section 3.

A.1. Mean-Field *XY* Model

Here we want to prove the crucial estimate (22), which we used in Section 2 to compute the index of the critical points for the mean-field XY model.

We recall that we want to compute the the number of negative eigenvalues of the Hessian matrix of the function $\mathcal{V}$, i.e., of the matrix H whose elements H_{ij} are

$$H_{ij} = \frac{\partial^2 \mathcal{V}}{\partial \varphi_i \partial \varphi_j} \qquad i, j = 1, \dots, N, \tag{A1}$$

where $\mathcal{V} = V/N$ and V is the potential energy of the mean-field XY model defined in Eq. (2). The diagonal elements of this matrix are

$$H_{ii} = d_i = \frac{1}{N}\left[(m_x + h) \cos \varphi_i + m_y \sin \varphi_i\right] - \frac{1}{N^2}, \tag{A2}$$

and the off-diagonal ones are

$$H_{ij} = -\frac{1}{N^2}(\sin \varphi_i \sin \varphi_j + \cos \varphi_i \cos \varphi_j). \tag{A3}$$

At the critical points of $\mathcal{V}$, the angles are either 0 or π, so that the sines are all zero and the cosines are ± 1. Moreover, since we are interested only in the signs of the eigenvalues of H and not in their absolute values, we multiply H by N in order to get rid of the $1/N$ factor in front of it. We can then write the matrix H (multiplied by N) as

$$H = D + B \tag{A4}$$

where D is a diagonal matrix,

$$D = \mathrm{diag}(\delta_i), \tag{A5}$$

whose elements δ are

$$\delta_i = (m_x + h) \cos \varphi_i, \tag{A6}$$

where the φ_i's ($i = 1,..., N$) are computed at the critical point, and the elements of B can be written in terms of a vector σ whose N elements are either 1 or -1:

$$b_{ij} = -\frac{1}{N}\sigma_i\sigma_j, \tag{A7}$$

where

$$\sigma_i = +1(-1) \qquad \text{if} \quad \varphi_i = 0(\pi). \tag{A8}$$

This, since when the angles are either 0 or π, the sines in Eq. (20) vanish, so that then

$$NH_{ij} = -\frac{1}{N}\cos\varphi_i \cos\varphi_j, \tag{A9}$$

and

$$\cos\varphi_i = \sigma_i. \tag{A10}$$

Having fixed the notation, our goal is to show that, at least when N is large, the number of negative eigenvalues of the full matrix H, i.e., the index of the critical point, can be conveniently approximated by the number of negative eigenvalues of D, that is, by the number of negative δ's. To do that, we proceed in two steps: (i) we show that the matrix B is of rank one (which implies that B has $N-1$ zero eigenvalues and only one nonzero eigenvalue), and (ii) we adapt a theorem due to Wilkinson[17] to this case, thus proving our assertion.

As to step (i), let us consider for example a case with $N = 3$, and the critical point corresponding to, say, $(\varphi_1, \varphi_2, \varphi_3) = (\pi, 0, 0)$. The vector σ is then

$$(\sigma_1, \sigma_2, \sigma_3) = (-1, 1, 1). \tag{A11}$$

Using Eq. (A7), the matrix B is

$$-\frac{1}{3}\begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}. \tag{A12}$$

We see that the second row is equal to the first multiplied by -1, and the same holds for the third row. This is true for any N, and is a consequence of Eq. (A7): any row of the matrix B is equal to another row multiplied by either $+1$ or -1. This means that $N-1$ rows are not linearly independent and that the rank of the matrix is one.

We have then proved that our Hessian matrix H is the sum of a diagonal matrix and of a matrix of rank one.

Let us now pass to step (ii). First, we recall a theorem of Wilkinson found in ref. 17:

Theorem A.1 (Wilkinson). Let A and B be $N \times N$ real symmetric matrices and let

$$C = A + B.$$

Let γ_i, α_i and β_i $(i = 1, 2,..., N)$ be the (real) eigenvalues of C, A, and B, respectively, arranged in non-increasing order, i.e.,

$$\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_N;$$
$$\alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_N;$$
$$\beta_1 \geqslant \beta_2 \geqslant \cdots \geqslant \beta_N.$$

Then

$$\gamma_{r+s-1} \leqslant \alpha_r + \beta_s \qquad \forall\, r+s-1 \leqslant N. \tag{A13}$$

Notice that we can also write

$$A = C + (-B), \tag{A14}$$

and since the eigenvalues of $-B$ arranged in non-increasing order are

$$-\beta_{N-i+1}$$

we can write

$$\alpha_{r+s-1} \leqslant \gamma_r - \beta_{N-s+1}. \tag{A15}$$

Now, we are interested in a special case, i.e., the case in which the matrix B is of rank one (has only one nonzero eigenvalue). What does Wilkinson's theorem say when applied to such a special case? We consider the two possible cases, namely:

(a) the nonzero eigenvalue is negative:

$$\beta_i = 0 \qquad \text{for} \quad i = 1, 2,..., N-1, \quad \beta_N = -\varrho;$$

(b) the nonzero eigenvalue is positive:

$$\beta_N = \varrho, \beta_i = 0 \qquad \text{for} \quad i = 2, 3, \ldots, N.$$

Case (a). Choosing $s = 1$ in Eq. (A13) we get $\beta_s = 0$, so that

$$\gamma_r \leqslant \alpha_r \qquad r = 1, \ldots, N, \tag{A16}$$

while choosing $s = 2$ in Eq. (A15) we get $-\beta N - s + 1 = 0$ again, whence

$$\alpha_{r+1} \leqslant \gamma_r \qquad r = 1, \ldots, N-1. \tag{A17}$$

Combining Eqs. (A16) and (A17) we obtain

$$\alpha_{r+1} \leqslant \gamma_r \leqslant \alpha_r \qquad r = 1, \ldots, N-1; \tag{A18}$$

$$\gamma_N \leqslant \alpha_N. \tag{A19}$$

We have thus shown that all the eigenvalues of C (except for the smallest one) are bounded between two successive eigenvalues of A. As to γ_N, we can only say that it is smaller than (or equal to) the smallest eigenvalue of A.

Case (b). Choosing $s = 2$ in Eq. (A13) we get $\beta_s = 0$, so that

$$\gamma_{r+1} \leqslant \alpha_r \qquad r = 1, \ldots, N-1, \tag{A20}$$

while choosing $s = 1$ in Eq. (A15) we obtain

$$\alpha_r \leqslant \gamma_r \qquad r = 1, \ldots, N. \tag{A21}$$

Combining Eqs. (A20) and (A21) we obtain

$$\alpha_r \leqslant \gamma_r \leqslant \alpha_{r-1} \qquad r = 2, \ldots, N; \tag{A22}$$

$$\gamma_1 \geqslant \alpha_1. \tag{A23}$$

We have thus shown again that all the eigenvalues of C (except, in this case, for the largest one) are bounded between two successive eigenvalues of A. As to γ_1, we can only say that it is larger than (or equal to) the smallest eigenvalue of A, α_1.

Let us now apply these results to our problem, i.e., to the computation of the number of negative eigenvalues of the matrix H in Eq. (A4). Denoting by η_i its eigenvalues, by δ_i those of D and by β_i those of B, we have

$$\beta_i = 0 \qquad \forall\, i \neq 1, N, \tag{A24}$$

and either

$$\beta_1 = 0, \qquad \beta_N = -\varrho,$$

or

$$\beta_1 = \varrho, \qquad \beta_N = 0.$$

At a given critical point, with n_π angles equal to π, the eigenvalues of D are (for the moment we do not order them)

$$\delta_i = m_x + h \qquad i = 1,..., N - n_\pi; \tag{A25}$$

$$\delta_i = -(m_x + h) \qquad i = N - n_\pi + 1,..., N. \tag{A26}$$

The x-component of the magnetization vector is given by

$$m_x = 1 - \frac{2n_\pi}{N} \tag{A27}$$

so that

$$m_x > 0 \qquad \text{if} \quad n_\pi \leqslant \frac{N}{2}, \tag{A28}$$

$$m_x < 0 \qquad \text{if} \quad n_\pi > \frac{N}{2}. \tag{A29}$$

Then, if the external field h is sufficiently small:
if $n_\pi \leqslant N/2$, then

$$\delta_i = m_x + h > 0 \qquad i = 1,..., N - n_\pi, \tag{A30}$$

$$\delta_i = -(m_x + h) < 0 \qquad i = N - n_\pi + 1,..., N, \tag{A31}$$

i.e., there are $N - n_\pi$ positive and n_π negative δ's;
else if $n_\pi \leqslant N/2$, then

$$\delta_i = -(m_x + h) > 0 \qquad i = 1,..., n_\pi, \tag{A32}$$

$$\delta_i = m_x + h < 0 \qquad i = n_\pi + 1,..., N, \tag{A33}$$

i.e., there are n_π positive and $N - n_\pi$ negative δ's.

Now we claim that, at least as N gets large, we can estimate the number of negative η's, i.e., the index of the critrical point, by saying that it is equal to the number of negative $\delta's$. More precisely, we claim that the error of our estimate is not larger than 1, i.e.,

$$\mathrm{index}(H) = \#(\eta < 0) = \#(\delta < 0) \pm 1. \tag{A34}$$

and as N gets large this error becomes obviously negligible. To prove this statement, let us consider the case in which $n_\pi < N/2$. We observe that we do not know whether we are in Case (a) or in Case (b), i.e., we do not know if the matrix B has a negative or a positive eigenvalue. But we can, anyway, try one of the two cases, say (a). Using Eqs. (A18) and (A19) we can then say that

$$\delta_{r+1} \leqslant \eta_r \leqslant \delta_r < 0 \qquad r = N - n_\pi + 1, \ldots, N-1, \tag{A35}$$

(note that these are $n_\pi - 1$ equations), and that

$$\eta_N \leqslant \delta_N < 0. \tag{A36}$$

Thus we conclude that the number of negative η's is just equal to that of negative δ's, i.e., n_π. If we guessed correctly the sign of the nonzero eigenvalue of B, then, our estimate is exact. But in case we guessed it wrong, i.e., if we were in Case (b) and not (a), by using Eqs. (A18) and (A19), we would have overestimated the number of negative η's by 1. Conversely, if we had used the equations of Case (b) in a situation which belonged to Case (a) we would have underestimated the index by 1. So, we conclude that the error of our estimate is always ± 1.

A.2. One-Dimensional *XY* Model

Here we want to discuss the details of the result reported in Eq. (36), i.e., that in the case of the one-dimensional XY model with nearest-neighbor interactions the index of the critical points equals the number n_d of "domain walls" in the configuration.

First of all, let us notice that in the present case the Hessian matrix H is tridiagonal, i.e., it can be written as

$$H = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \beta_{N-2} & \alpha_{N-1} & \beta_{N-1} \\ 0 & \cdots & 0 & 0 & \beta_{N-1} & \alpha_N \end{pmatrix} \tag{A37}$$

where, assuming free boundary conditions,

$$\alpha_1 = \cos(\varphi_2 - \varphi_1) + h\cos(\varphi_1); \tag{A38a}$$

$$\alpha_i = \cos(\varphi_{i+1} - \varphi_i) + \cos(\varphi_i - \varphi_{i-1}) + h\cos(\varphi_i), \qquad i = 2, \dots, N-1; \tag{A38b}$$

$$\alpha_N = \cos(\varphi_N - \varphi_{N-1}) + h\cos(\varphi_N), \tag{A38c}$$

and

$$\beta_i = -\cos(\varphi_{i+1} - \varphi_i), \qquad i = 1, \dots, N-1. \tag{A39}$$

Since at critical points $\varphi_i = 0$ or π, we have that for any i and for any critical point

$$\beta_i = \pm 1 \tag{A40}$$

while the diagonal elements α_i are

$$\alpha_1 = 1 \pm h; \tag{A41a}$$

$$\alpha_i = 2 \pm h, \qquad i = 2, \dots, N-1; \tag{A41b}$$

$$\alpha_N = 1 \pm h, \tag{A41c}$$

if there are no domain walls, i.e., if $n_d = 0$, while they can assume also the values $\pm h$ and $-2 \pm h$ ($-1 \pm h$ if $i = 1$ or $i = N$) if $n_d \neq 0$, i.e., if there are domain walls.

Let us now prove that $n_d \neq 0$ is a *necessary* condition for the presence of negative eigenvalues of the Hessian, i.e., for a nonvanishing index of a critical point. To do that, we recall a theorem due to Gershgorin (see, e.g., ref. 17), which, in the simple case of a real symmetric matrix, can be stated as follows:

Theorem 1.2 (Gershgorin). Let A be a real $n \times n$ symmetric matrix whose elements are a_{ij}, and let

$$r_i = \sum_{j \neq i} |a_{ij}|, \qquad i = 1, \dots, n;$$

the eigenvalues of A lie in the intervals

$$X_i = \{x \in \mathbb{R} : |x - a_{ii}| < r_i\};$$

if m of the X_i form a disjoint set, then precisely m eigenvalues (counted with their multiplicity) lie in it.

In our case, due to Eq. (A40), at any critical point we have

$$r_1 = r_N = 1; \tag{A42a}$$

$$r_i = 2, \qquad i = 2, \ldots, N-1, \tag{A42b}$$

so that, if $n_d = 0$ and $h \to 0$, Eqs. (A41) and Gershgorin's theorem imply that all the eigenvalues lie in the interval $|x-2| < 2$, so that there are no negative eigenvalues and the index is zero. On the other hand, if $n_d \neq 0$ and $h \to 0$, then the intervals X_i are either $|x| < 2$, or $|x+2| < 2$, hence the eigenvalues lie in the interval $(-4, 2)$, so that the index can be nonvanishing. However, Gershgorin's theorem is useless to compute the number of negative eigenvalues, because the intervals X_i overlap each other, thus the eigenvalues cannot be localized more strictly.

Anyway, the fact that the Hessian is tridiagonal allows us to compute directly its characteristic polynomial $\det(H - \lambda I)$, whose roots $\lambda_1, \ldots, \lambda_N$ are the eigenvalues, by means of a recurrence formula. Let

$$p_0(\lambda) = 1; \tag{A43a}$$

$$p_1(\lambda) = \alpha_1 - \lambda; \tag{A43b}$$

$$p_k(\lambda) = (\alpha_k - \lambda)\, p_{k-1}(\lambda) - \beta_{k-1}^2 p_{k-2}(\lambda) \tag{A43c}$$

then, since

$$p_k(\lambda) = \det \begin{pmatrix} \alpha_1 - \lambda & \beta_1 & 0 & 0 & \cdots & 0 \\ \beta_1 & \alpha_2 - \lambda & \beta_2 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \beta_{k-2} & \alpha_{k-1} - \lambda & \beta_{k-1} \\ 0 & \cdots & 0 & 0 & \beta_{k-1} & \alpha_k - \lambda \end{pmatrix},$$

$$k = 2, \ldots, N, \tag{A44}$$

the characteristic polynomial of H is given by $p_N(\lambda)$. Since at the critical points all the β's are ± 1 – see Eqs. (A40), we have that

$$p_0(\lambda) = 1; \tag{A45a}$$

$$p_1(\lambda) = \alpha_1 - \lambda; \tag{A45b}$$

$$p_k(\lambda) = (\alpha_k - \lambda)\, p_{k-1}(\lambda) - p_{k-2}(\lambda) \tag{A45c}$$

so that the characteristic polynomial $p_N(\lambda)$ depends only on the α's. Moreover, the following theorem holds (see, e.g., ref. 21):

Theorem A.3. Let H be a tridiagonal symmetric matrix defined as in Eq. (A37). Define the sequence

$$\{p_0(\lambda), p_1(\lambda),..., p_N(\lambda)\} \tag{A46}$$

as in Eq. (A43c); then the number of sign changes in the sequence (with the rule that if $p_i(\lambda) = 0$ then it has the opposite sign of $p_{i-1}(\lambda)$) equals the number of eigenvalues of H which are less than or equal to λ.

Then the number n_c of sign changes in the sequence

$$\{p_0(0), p_1(0),..., p_N(0)\} \tag{A47}$$

equals the number of negative eigenvalues, i.e., the index of the critical point because no eigenvalues are zero. If one puts $h = 0$, then there is one eigenvalue which becomes zero at any critical point, so that the index equals $n_c - 1$, but in this case one easily sees by direct computation (which can be performed exactly on a computer at any N because in this case the α's are integer numbers) that $n_d = n_c - 1$, so that one finds the result reported in Eq. (36).

ACKNOWLEDGMENTS

We warmly thank R. Franzosi, L. Spinelli, and G. Vezzosi for very helpful discussions and suggestions. This work is part of the INFM PAIS *Equilibrium and Non-Equilibrium Dynamics of Condensed Matter Systems*. EGDC gratefully acknowledges support from the Office of Basic Engineering Science of the US Department of Energy, under Grant No. DE-FG 02-88-ER 13847, and from the IS-Sabbatical of the INFM.

REFERENCES

1. C. N. Yang and T. D. Lee, *Phys. Rev.* **87**:404 (1952); T. D. Lee and C. N. Yang, *Phys. Rev.* **87**:410 (1952).
2. D. Ruelle, *Statistical Mechanics: Rigorous Results* (World Scientific, Singapore, 1999).
3. See, e.g., H. O. Georgii, *Gibbs Measures and Phase Transitions* (de Gruyter, New York, 1988).
4. D. H. E. Gross, *Microcanonical Thermodynamics, Phase Transitions in Small Systems* (World Scientific, Singapore, 2001).
5. L. Caiani, L. Casetti, C. Clementi, and M. Pettini, *Phys. Rev. Lett.* **79**:4361 (1997).
6. R. Franzosi, L. Casetti, L. Spinelli, and M. Pettini, *Phys. Rev. E* **60**:R5009 (1999).
7. L. Casetti, E. G. D. Cohen, and M. Pettini, *Phys. Rev. Lett.* **82**:4160 (1999).

8. R. Franzosi, M. Pettini, and L. Spinelli, *Phys. Rev. Lett.* **84**:2774 (2000).
9. L. Casetti, M. Pettini, and E. G. D. Cohen, *Phys. Rep.* **337**:237 (2000).
10. M. Cerruti-Sola, C. Clementi, and M. Pettini, *Phys. Rev. E* **61**:5171 (2000).
11. M. Nakahara, *Geometry, Topology and Physics* (Adam Hilger, Bristol, 1991).
12. J. Milnor, *Morse Theory* (Princeton University Press, Princeton, 1951).
13. R. S. Palais and C. Terng, *Critical Point Theory and Submanifold Geometry* (Springer, NY, 1988).
14. R. Franzosi, M. Pettini, and L. Spinelli, `cond-mat/0104110`, and in preparation.
15. L. Casetti, E. G. D. Cohen, and M. Pettini, *Phys. Rev. E* **65**:036112 (2002).
16. M. Antoni and S. Ruffo, *Phys. Rev. E* **52**:2361 (1995).
17. J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Clarendon Press, Oxford, 1965).
18. P. G. Debenedetti and F. H. Stillinger, *Nature* **410**:259 (2001).
19. L. Angelani *et al.*, *Phys. Rev. Lett.* **85**:5356 (2000); A. Cavagna, I. Giardina, and G. Parisi, *J. Phys. A: Math. Gen.* **34**:5317 (2001); T. S. Grigera, A. Cavagna, I. Giardina, and G. Parisi, *Phys. Rev. Lett.* **88**:055502 (2002); R. M. C. de Almeida, N. Lemke, and I. A. Campbell, `cond-mat/0003351`.
20. B. A. Dubrovin, A. T. Fomenko, and S. P. Novikov, *Modern Geometry-Methods and Applications* (Parts I, II, and III, Springer, NY, 1985).
21. G. H. Golub and C. F. Van Loan, *Matrix Computations* (Johns Hopkins University Press, Baltimore, 1996).
22. M. Spivak, *Comprehensive Introduction to Differential Geometry* (Publish or Perish, Berkeley, 1979).