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Topological aspects of geometrical signatures of phase transitions

Roberto Franzosi,[1,2,*] Lapo Casetti,[3,†] Lionel Spinelli,[2,4,‡] and Marco Pettini[2,5,§]
[1]*Dipartimento di Fisica, Università di Firenze, Largo Enrico Fermi 2, 50125 Firenze, Italy*
[2]*Istituto Nazionale per la Fisica della Materia, Unità di Ricerca di Firenze, Firenze, Italy*
[3]*Istituto Nazionale per la Fisica della Materia, Dipartimento di Fisica, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy*
[4]*Centre de Physique Théorique du CNRS, Luminy Case 907, 13288 Marseille Cedex 9, France*
[5]*Osservatorio Astrofisico di Arcetri, Largo Enrico Fermi 5, 50125 Firenze, Italy*

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Certain geometric properties of submanifolds of configuration space are numerically investigated for classical lattice φ^4 models in one and two dimensions. Peculiar behaviors of the computed geometric quantities are found only in the two-dimensional case, when a phase transition is present. The observed phenomenology strongly supports, though in an indirect way, a recently proposed *topological conjecture* about a topology change of the configuration space submanifolds as counterpart to a phase transition. [S1063-651X(99)50311-5]

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In statistical mechanics phase transitions are associated with the appearence of the so-called Yang-Lee (real) zeros [1] of the grand-partition function entailing singular temperature dependence of thermodynamic observables. However, in the Yang-Lee theory the necessary conditions for the existence of real zeros remain unspecified. It has recently been suggested [2,3] that the thermodynamic singularities might have their deep origin in some major topological change in configuration space, i.e., in a nontrivial structure of the *support* of the equilibrium statistical measure.

This *topological conjecture* [4] has been put forward heuristically within the framework of a numerical investigation of the Hamiltonian dynamical counterpart of phase transitions. An interesting outcome of such investigations was the clear evidence of a peculiar temperature behavior of the largest Lyapunov exponent at the phase transition point. This was observed in lattice scalar and vector φ^4 models [3,5], in two- and three-dimensional (2D and 3D) XY models [2], in the Θ transition of homopolymeric chains [6], and — analytically — in the mean-field XY model [7]. Moreover, in light of a Riemannian geometrization of Hamiltonian dynamics — where Lyapunov exponents are related to average curvature properties of submanifolds of configuration space [8–10] — the temperature dependence of abstract geometric observables has also been investigated. Among these geometric observables, the averages of curvature fluctuations (that enter the analytic formula for the largest Lyapunov exponent [10]) exhibit a cusplike pattern. The peak coincides with the phase transition point. Similar peaks of curvature fluctuations have been reproduced in abstract geometric models (families of surfaces of $\mathbb{R}^3$ where the variation of a parameter leads to a change in the topological genus), whence the *heuristic* argument about the topological meaning of the peaks of configuration-space-curvature fluctuations at a phase transition. These fluctuations have been obtained as time averages, computed along the dynamical trajectories of the Hamiltonian systems under investigation. Now, time averages of geometric observables are usually found to be in excellent agreement with ensemble averages [2,3,10,11]; therefore, one could argue that the mentioned singularlike patterns of the averages of geometric observables are simply the precursors of truly singular patterns due to the fact that the measures of all the statistical ensembles tend to become singular in the limit $N\to\infty$ when a phase transition is present. In other words, geometric observables, like any other ''honest'' observable, already at finite N would feel the eventually singular character of the statistical measures, and if this were the true explanation we could not attribute the cusplike patterns of curvature fluctuations to special geometric features of configuration space. Hence the motivation behind the present paper. Our goal is to elucidate this important point by working out *purely geometric* information about the submanifolds (to be specified below) of configuration space, *independently* of the statistical measures. In the present paper a step forward is made toward supporting the *topological conjecture* mentioned above.

Our geometrical framework is the configuration space M of systems whose degrees of freedom are uncostrained and are real numbers, thus $M=\mathbb{R}^N$.

Our statistical framework is the canonical ensemble whose volume in M is given by the configurational partition function $Z_C=\int\Pi_{i=1}^N dq_i \exp[-\beta V(q)]$, where $q=(q_1,\dots,q_N)\in\mathbb{R}^N$ and $1/\beta$ is the temperature. Finally, our topological framework is elementary Morse theory [12,13]. Let us here recall its basic idea with the help of Fig. 1. The ''U-shaped'' cylinder of Fig. 1 is the ambient manifold M where a function $V:M\mapsto\mathbb{R}$, smooth and bounded below, is defined to be the height of any point of M with respect to the ''ground plane.'' For any given value u of the function V two

*Also at INFN, Sezione di Firenze, Firenze, Italy. Electronic address: franzosi@fi.infn.it

†Electronic address: lapo@polito.it

‡Present address: Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, 50125 Firenze, Italy. Electronic address: spinelli@arcetri.astro.it

§Also at INFN, Sezione di Firenze, Firenze, Italy. Electronic address: pettini@arcetri.astro.it

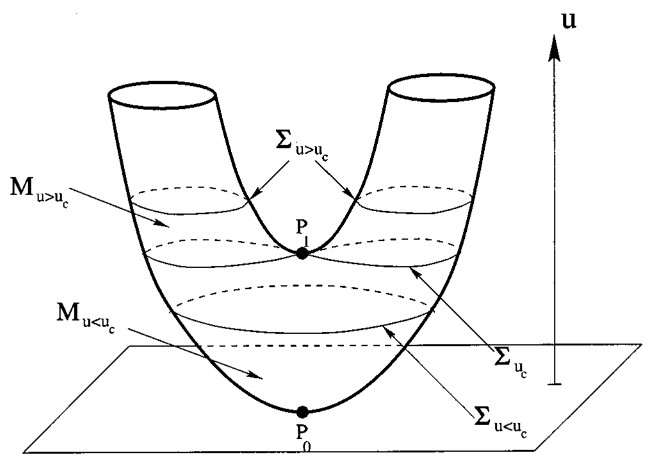

FIG. 1. Illustration of the relationship between topology and critical points. The U-shaped manifold M is born at P_0. The level surfaces Σ_u and the parts of M below them — M_u — change topology when u exceeds the height of the critical point P_1.

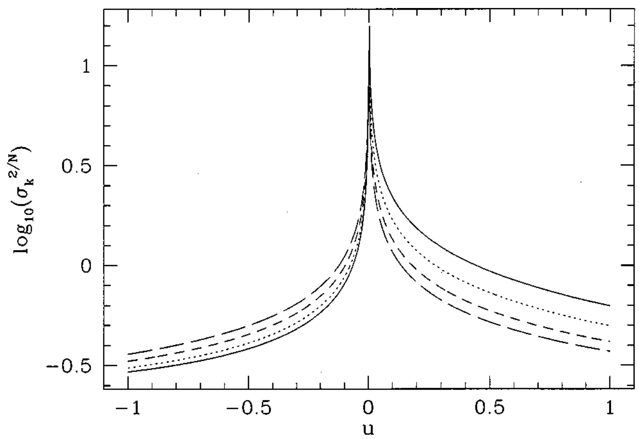

FIG. 2. Variance of Gauss curvature vs u close to a critical point. $\sigma_K^{2/N}$ is reported because it is dimensionally homogeneous to the scalar curvature. Here $N=\dim(\Sigma_u)=100$, and Morse indexes are $k=1,15,33,48$, represented by solid, dotted, dashed, long-dashed lines, respectively.

kinds of submanifolds are determined: the level sets Σ_u of all the points $x\in M$ for which $V(x)=u$, and M_u, the part of M below the level u, i.e., the set of all points $x\in M$ such that $V(x)\leqslant u$. The remarkable fact about the Morse theory is that from the knowledge of all the critical points of V, i.e., those points where $\nabla V=0$, and of their Morse indexes, i.e., the number of negative eigenvalues of the Hessian of V, one can infer the topological structure of the manifolds M_u, provided that the critical points are nondegenerate, i.e., with nonvanishing eigenvalues of the Hessian of V. Two such points are marked in Fig. 1, at the bottom of M and at some intermediate level u_c for which Σ_{u_c} is an figure-eight-shaped curve. It is evident from Fig. 1 that the manifolds $M_{u<u_c}$ are *not diffeomorphic* to the manifolds $M_{u>u_c}$: the former are homeomorphic to a disk and the latter are homeomorphic to a cylinder. The same thing happens (in general) to the boundaries Σ_u that here are circles for $u<u_c$ and become the topological union of two circles for $u>u_c$. This simple example displays the general fact that *passing a critical level of a Morse function is in one-to-one relation with a topology change*. A critical level is a surface Σ_u that contains one or more critical points.

Let us now consider the configuration space $M=\mathbb{R}^N$ of a physical system and its potential V as the Morse function. The interesting things are supposed to occur below some large value $\overline{u}$ so that the corresponding (large) subset $\overline{M}\subset M$ is compact. Then $\overline{M}$ and all its submanifolds M_u are given a Riemannian metric g. On all these manifolds (M_u,g) there is a standard invariant volume element: $d\eta=\sqrt{\det(g)}dq^1\cdots dq^N$.

In order to study the topology of the family $\{(M_u,g)\}$ we should find, analytically or numerically, all the critical points of V. At large N this is a formidable task; therefore, we have approached this problem as follows. Generalizing a simple geometric example reported in [2,3], we have computed the total degree of second variation σ_K^2 of the Gaussian curvature, i.e., $\sigma_K^2=\langle K_G^2\rangle_{\Sigma_u}-\langle K_G\rangle_{\Sigma_u}^2$, where $\langle\ \rangle$ stands for integration over the surface Σ_u, as a function of u in the neighborhood of a critical point. This is possible in general, regardless of the precise form of the potential V, because any Morse function can be parametrized in the neighborhood of a critical point, located at $x_0\in M$, by means of the so-called *Morse chart*, i.e., a system of local coordinates $\{x_i\}$ such that $V(x)=V(x_0)-\Sigma_{i=1}^k x_i^2+\Sigma_{i=k+1}^N x_i^2$ (k is the Morse index). Then standard formulas for Gauss curvature of hypersurfaces of $\mathbb{R}^N$ [14] can be used to explicitly work out K_G and σ_K^2. The intersection of a hypersphere of unit radius — centered around $u=0$ (the critical point) — with each Σ_u is used to bound the domain of integration. The numerically tabulated results are reported in Fig. 2 and show that σ_K^2 develops a sharp, singular peak as the critical surface is approached. It seems, therefore, reasonable to apply this geometric probing of the presence of critical points, and hence of topology changes, to the study of possible topology changes of the manifolds (M_u,g). In fact, the properties of the manifolds M_u are closely related to those of the hypersurfaces $\{\Sigma_u\}_{u\leqslant u_c}$, as can be inferred from the equation $\int_{M_u} f d\eta=\int_0^u dv\int_{\Sigma_v} f|_{\Sigma_v} d\omega/\|\nabla V\|$, where $d\omega$ is the induced measure on Σ_v and f a generic function [15]. The surface Σ_{u_c} defined by $V(x)=u_c$ is a degenerate quadric; therefore in its vicinity some of the principal curvatures [14] of the surfaces $\Sigma_{u\simeq u_c}$ tend to diverge. Such a divergence is generally detected by any function of the principal curvatures and thus, for practical computational reasons, instead of Gauss curvature (which is the product of all the principal curvatures) we shall consider the total second variation of the *scalar* curvature $\mathcal{R}$ (i.e., the sum of all the possible products of two principal curvatures) of the manifolds (M_u,g), according to the definition

$$\sigma_{\mathcal{R}}^2(u)=[\mathrm{Vol}(M_u)]^{-1}\int_{M_u} d\eta(\mathcal{R}-\varrho_u)^2, \tag{1}$$

$$\varrho_u=[\mathrm{Vol}(M_u)]^{-1}\int_{M_u} d\eta\,\mathcal{R}, \tag{2}$$

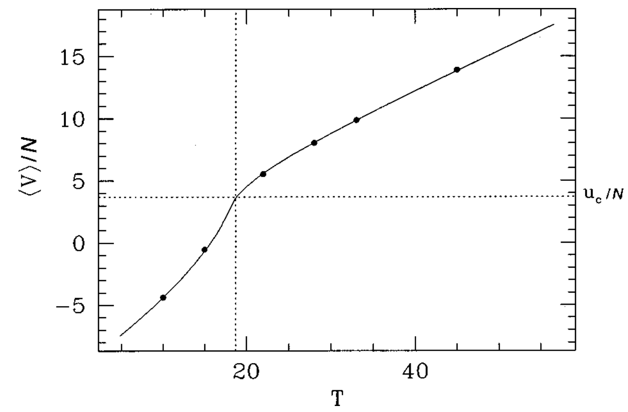

FIG. 3. Average potential energy density vs temperature for the 2D lattice φ^4 model. Lattice size $N=20\times 20$. The solid line, made of 200 points, refers to time averages. Full circles represent Monte Carlo estimates of canonical ensemble averages. The dotted lines locate the phase transition.

with $\mathcal{R}=g^{kj}R^l_{klj}$, where R^l_{kij} is the Riemann curvature tensor [16], and $\mathrm{Vol}(M_u)=\int_{M_u}d\eta$.

Let us now consider the family of submanifolds (M_u,g) associated with the so-called φ^4 model, on a d-dimensional lattice $\mathbb{Z}^d$, described by the potential function

$$V=\sum_{\alpha\in\mathbb{Z}^d}\left(-\frac{\mu^2}{2}q_\alpha^2+\frac{\lambda}{4!}q_\alpha^4\right)+\sum_{\langle\alpha\beta\rangle\in\mathbb{Z}^d}\frac{1}{2}J(q_\alpha-q_\beta)^2, \tag{3}$$

where $\langle\alpha\beta\rangle$ stands for nearest-neighboring sites. We consider $d=1,2$; this system has a discrete $\mathbb{Z}_2$ symmetry and short-range interactions; therefore, in $d=1$ there is no phase transition whereas in $d=2$ there is a symmetry-breaking transition (this system has the same universality class of the 2D Ising model).

The potential in Eq. (3) defines the subsets M_u of configuration space. These subsets are given the structure of Riemannian manifolds (M_u,g) by endowing all of them with the *same* metric tensor g. However, since we want to know something about the topology of these manifolds, the choice of the metric g is arbitrary. We have therefore chosen three different types of metrics, one conformally flat and the others nonconformal, according to a compromise between simplicity and nontriviality. (i) $g^{(1)}_{\mu\nu}=[A-V(q)]\delta_{\mu\nu}$, i.e., a conformal deformation of the Euclidean flat metric $\delta_{\mu\nu}$, $A>0$ is an arbitrary constant larger than $\overline{u}$. (ii) and (iii) $g^{(2)}_{\mu\nu}$ and $g^{(3)}_{\mu\nu}$ are nonconformal metrics defined by

$$(g^{(k)}_{\mu\nu})=\begin{pmatrix} f^{(k)} & 0 & 1\\ 0 & \mathbb{I} & 0\\ 1 & 0 & 1\end{pmatrix},\quad k=2,3, \tag{4}$$

where $\mathbb{I}$ is the $N-2$-dimensional identity matrix, $g^{(2)}$ is obtained by setting $f^{(2)}=(1/N)\Sigma_{\alpha\in\mathbb{Z}^d}q_\alpha^4+A$ and $g^{(3)}$ by setting $f^{(3)}=(1/N)\Sigma_{\alpha\in\mathbb{Z}^d}q_\alpha^6+A$, with $A>0$, and α labels the N lattice sites of a linear chain $(d=1)$ or of a square lattice $(d=2,\ N=n\times n)$. Simple algebra [16] yields the scalar curvature function for each metric:

$$\mathcal{R}^{(1)}=(N-1)\left[\frac{\Delta V}{(A-V)^2}-\frac{\|\nabla V\|^2}{(A-V)^3}\left(\frac{N}{4}-\frac{3}{2}\right)\right], \tag{5}$$

$$\mathcal{R}^{(k)}=\frac{1}{(f^{(k)}-1)}\left[\frac{\|\tilde\nabla f^{(k)}\|^2}{2(f^{(k)}-1)}-\tilde\Delta f^{(k)}\right],\quad k=2,3, \tag{6}$$

where ∇ and Δ are Euclidean gradient and Laplacian, respectively; $\tilde\nabla$ and $\tilde\Delta$ do not contain the derivatives $\partial/\partial q_\alpha$ with $\alpha=1$ $(d=1)$ or $\alpha=(1,1)$ $(d=2)$.

We constructed an *ad hoc* Monte Carlo algorithm to sample the geometric measure $d\eta$ by means of the standard "importance sampling" method [17], then we applied it to the computation of $\sigma^2_{\mathcal{R}}(u)$, given by Eq.(2), for the one- and two-dimensional lattice φ^4 models defined in Eq. (3) with the following choice of parameters: $\lambda=0.6$, $\mu^2=2$, $J=1$. The values of $\mathcal{R}$ are computed according to Eqs. (5) and (6).

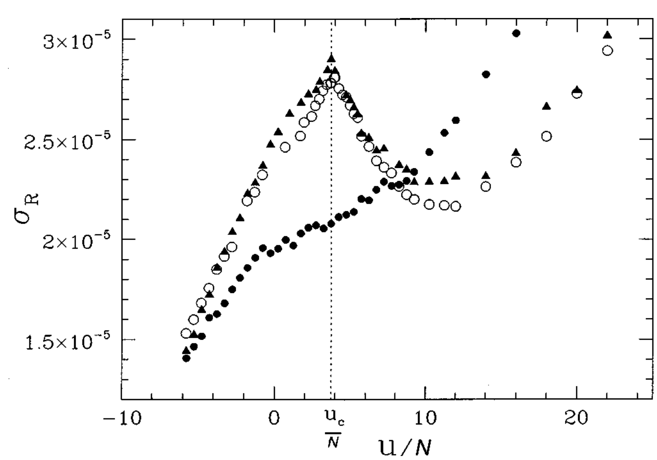

FIG. 4. Variance of the scalar curvature of M_u vs u/N computed with the metric $g^{(1)}$. Full circles correspond to the 1D-φ^4 model with $N=400$. Open circles refer to the 2D-φ^4 model with $N=20\times 20$ lattice sites, and full triangles refer to 40×40 lattice sites (whose values are rescaled for graphic reasons).

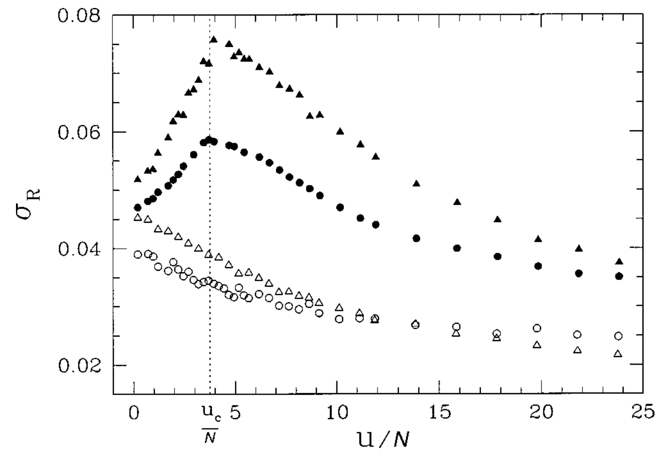

FIG. 5. Variance of the scalar curvature of M_u vs u/N computed for the φ^4 model with metric $g^{(2)}$ in 1D, $N=400$ (open triangles); metric $g^{(2)}$ in 2D, $N=20\times 20$ (full triangles); metric $g^{(3)}$ in 1D, $N=400$ (open circles); metric $g^{(3)}$ in 2D, $N=20\times 20$ (full circles).

In order to locate the phase transition that occurs in the two-dimensional case, we have computed $\langle V \rangle$ vs T by means of both Monte Carlo averaging with the canonical configurational measure and Hamiltonian dynamics (by adding to V a standard kinetic energy term). In the latter case the temperature T is given by the average kinetic energy per degree of freedom, and $\langle V \rangle$ is obtained as a time average. Figure 3 shows perfect agreement between time and ensemble averages; thus, we worked out Fig. 3 by computing 200 time averages because they converge much faster than ensemble averages. The phase transition point is well visible at $u_c/N = \langle V \rangle/N \simeq 3.75$.

In Figs. 4 and 5 we synoptically report the patterns of $\sigma^2_{\mathcal{R}}(u)$ for the one- and two-dimensional cases obtained at different lattice sizes with $g^{(1)}$ (Fig. 4), and obtained at a given lattice size [18] with $g^{(2,3)}$ (Fig. 5). Peaks of $\sigma^2_{\mathcal{R}}(u)$ appear at u_c — the value of $\langle V \rangle$ at the phase transition point — in the two-dimensional case, whereas only monotonic patterns are found in the one-dimensional case, where no phase transition is present.

''Singular,'' cuspy patterns of $\sigma^2_{\mathcal{R}}(u)$ (with the implications that such attributes can have regarding numerical results) are found *independently* of any possible statistical mechanical effect, and *independently* of the geometric structure given to the family $\{M_u\}$ by the metric tensors chosen. Though within the very evident limits of numerical simulations and of a limited choice of different metrics, our results suggest that the ''singular'' patterns are most likely to have their origin at a deeper level than the geometric one, i.e., at the topological level. Hence the observed phenomenology strongly hints that some *major* change in the topology of the configuration-space submanifolds $\{M_u\}$ occurs in correspondence with a second-order phase transition [19]. Finally, the expression ''*major* topology change'' is meant to suggest that a change of the cohomological type of the M_u — or Σ_u — might well be a necessary but not sufficient condition for a phase transition, and that in any case some ''big'' change has to occur.

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