Topology and Phase Transitions: Paradigmatic Evidence

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We report upon the numerical computation of the Euler characteristic χ (a topologic invariant) of the equipotential hypersurfaces Σ_v of the configuration space of the two-dimensional lattice φ^4 model. The pattern $\chi(\Sigma_v)$ versus v (potential energy) reveals that a major topology change in the family $\{\Sigma_v\}_{v\in\mathbb{R}}$ is at the origin of the phase transition in the model considered. The direct evidence given here—of the relevance of topology for phase transitions—is obtained through a general method that can be applied to any other model.

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Suitable topology changes of equipotential submanifolds of configuration space can entail thermodynamic phase transitions. This is the novel result of the present Letter. The method we use, though applied here to a particular model, is of general validity and it is of prospective interest to the study of phase transitions in those systems that challenge the conventional approaches, as might be the case of finite systems (like atomic and molecular clusters), of off-lattice polymers and proteins, of glasses, and in general of amorphous and disordered materials. Let us begin by giving a theoretical argument and then proceed by numerically proving its truth for the 2D lattice φ^4 model. Consider classical many particle systems described by standard Hamiltonians

$$H(p,q) = \sum_{i=1}^{N} \frac{1}{2}\, p_i^2 + V(q)\,, \tag{1}$$

where the $(p,q) \equiv (p_1,\ldots,p_N,q_1,\ldots,q_N)$ coordinates assume *continuous* [1] values and $V(q)$ is bounded below. The statistical behavior of physical systems described by Hamiltonians as in Eq. (1) is encompassed, in the canonical ensemble, by the partition function in phase space

$$\begin{aligned} Z_N(\beta) &= \int \prod_{i=1}^{N} dp_i\, dq_i\, e^{-\beta H(p,q)} \\ &= \left(\frac{\pi}{\beta}\right)^{N/2} \int \prod_{i=1}^{N} dq_i\, e^{-\beta V(q)} \\ &= \left(\frac{\pi}{\beta}\right)^{N/2} \int_0^\infty dv\, e^{-\beta v} \int_{\Sigma_v} \frac{d\sigma}{\|\nabla V\|}\,, \end{aligned} \tag{2}$$

where the last term is written using a co-area formula [2], and v labels the equipotential hypersurfaces Σ_v of configuration space, $\Sigma_v = \{(q_1,\ldots,q_N) \in \mathbb{R}^N | V(q_1,\ldots,q_N) = v\}$.

Equation (2) shows that for Hamiltonians (1) the relevant statistical information is contained in the canonical configurational partition function $Z_N^C = \int \prod dq_i \times \exp[-\beta V(q)]$. Remarkably, Z_N^C is decomposed—in the last term of Eq. (2)—into an infinite summation of geometric integrals, $\int_{\Sigma_v} d\sigma/\|\nabla V\|$, defined on the $\{\Sigma_v\}_{v\in\mathbb{R}}$. Once the microscopic interaction potential $V(q)$ is given, the configuration space of the system is automatically foliated into the family $\{\Sigma_v\}_{v\in\mathbb{R}}$ of these equipotential hypersurfaces. Now, from standard statistical mechanical arguments we know that, at any given value of the inverse temperature β, the larger the number N of particles the closer to $\Sigma_v \equiv \Sigma_{u_\beta}$ are the microstates that significantly contribute to the averages—computed through $Z_N(\beta)$—of thermodynamic observables. The hypersurface Σ_{u_β} is the one associated with $u_\beta = (Z_N^C)^{-1} \int \prod dq_i\, V(q) e^{-\beta V(q)}$, the average potential energy computed at a given β. Thus, at any β, if N is very large the effective support of the canonical measure shrinks very close to a single $\Sigma_v = \Sigma_{u_\beta}$. Hence, and on the basis of what we found in [3–5], let us make explicit the following hypothesis.

Topological hypothesis.—The basic origin of a phase transition lies in a suitable topology change of the $\{\Sigma_v\}$, *occurring at some* v_c. *This topology change induces the singular behavior of the thermodynamic observables at a phase transition.*

By change of topology we mean that $\{\Sigma_v\}_{v<v_c}$ are *not diffeomorphic* to the $\{\Sigma_v\}_{v>v_c}$ [6]. In other words, the claim is that the canonical measure should "feel" a big and sudden change—if any—of the topology of the equipotential hypersurfaces of its underlying support, the consequence being the appearance of the typical signals of a phase transition, i.e., almost singular (at finite N) energy or temperature dependences of the averages of appropriate observables. The larger N, the narrower is the effective support of the measure and hence the sharper can be the mentioned signals, until true singularities appear in the $N \to \infty$ limit. This point of view has the interesting consequence that—also at finite N—in principle *different* mathematical objects, i.e., manifolds of different cohomology type, could be associated to *different* thermodynamical phases, whereas from the point of view of measure theory [7] the only mathematical property available to signal the appearance of a phase transition is the loss of analyticity of the grand-canonical and canonical averages, a fact which is compatible with analytic statistical measures only in the mathematical $N \to \infty$ limit.

In order to prove or disprove the conjectured role of topology, we have to explicitly work out adequate information about the topology of the members of the family $\{\Sigma_v\}_{v\in\mathbb{R}}$ for some given physical system. Below it is shown how this goal is practically achieved by means of numerical computations. As it is conjectured that the counterpart of a phase transition is a breaking of diffeomorphicity among the surfaces Σ_v, it is appropriate to choose a *diffeomorphism invariant* to probe if and how the topology of the Σ_v changes as a function of v. This is a very challenging task because we have to deal with high-dimensional manifolds. Fortunately a topological invariant exists whose computation is feasible, yet demands a big effort.

This is the *Euler characteristic*, a diffeomorphism invariant, expressing fundamental topological information [8]. In order to make the reader acquainted with it, we remind one that a way to analyze a geometrical object is to fragment it into other more familiar objects and then to examine how these pieces fit together. Take, for example, a surface Σ in the Euclidean three dimensional space. Slice Σ into pieces that are curved triangles (this is called a triangulation of the surface). Then count the number F of faces of the triangles, the number E of edges, and the number V of vertices on the tesselated surface. Now, no matter how we triangulate a compact surface Σ, $\chi(\Sigma) = F - E + V$ will always equal a constant which is characteristic of the surface and which is invariant under diffeomorphisms $\phi\colon \Sigma \to \Sigma'$. This is the Euler characteristic of Σ. At higher dimensions this can be again defined by using higher-dimensional generalizations of triangles (simplexes) and by defining the Euler characteristic of the n-dimensional manifold Σ to be

$$\chi(\Sigma) = \sum_{k=0}^{n} (-1)^k (\text{No. of “faces of dimension } k\text{”}) . \quad (3)$$

In differential topology a more standard definition of $\chi(\Sigma)$ is

$$\chi(\Sigma) = \sum_{k=0}^{n} (-1)^k b_k(\Sigma) , \quad (4)$$

where also the numbers b_k—the Betti numbers of Σ—are diffeomorphism invariants [9]. While it would be hopeless to try to practically compute $\chi(\Sigma)$ from Eq. (4) in the case of nontrivial physical models at large dimension, there is a possibility given by a powerful theorem, the Gauss-Bonnet-Hopf theorem, that relates $\chi(\Sigma)$ with the total Gauss-Kronecker curvature of the manifold, i.e., [10]

$$\chi(\Sigma) = \gamma \int_{\Sigma} K_G \, d\sigma \quad (5)$$

which is valid for even dimensional hypersurfaces of Euclidean spaces $\mathbb{R}^N$ [here $\dim(\Sigma) = n \equiv N - 1$], and where $\gamma = 2/\mathrm{Vol}(\mathbb{S}_1^n)$ is twice the inverse of the volume of an n-dimensional sphere of unit radius; K_G is the Gauss-Kronecker curvature of the manifold; $d\sigma = \sqrt{\det(g)}\, dx^1\, dx^2 \cdots dx^n$ is the invariant volume measure of Σ, and g is the Riemannian metric induced from $\mathbb{R}^N$. Let us briefly sketch the meaning and definition of the Gauss-Kronecker curvature.

The study of the way in which an n surface Σ curves around in $\mathbb{R}^N$ is measured by the way the normal direction changes as we move from point to point on the surface. The rate of change of the normal direction $\boldsymbol{\xi}$ at a point $x \in \Sigma$ in direction $\mathbf{v}$ is described by the *shape operator* $L_x(\mathbf{v}) = -\nabla_{\mathbf{v}}\xi$, where $\mathbf{v}$ is a tangent vector at x and $\nabla_{\mathbf{v}}$ is the directional derivative, hence $L_x(\mathbf{v}) = -(\nabla\xi_1 \cdot \mathbf{v}, \ldots, \nabla\xi_{n+1} \cdot \mathbf{v})$; gradients and vectors are represented in $\mathbb{R}^N$. As L_x is an operator of the tangent space at x into itself, there are n independent eigenvalues [11] $\kappa_1(x), \ldots, \kappa_n(x)$ which are called the principal curvatures of Σ at x. Their product is the Gauss-Kronecker curvature: $K_G(x) = \Pi_{i=1}^n \kappa_i(x) = \det(L_x)$. The practical computation of K_G for the equipotential hypersurfaces Σ_v proceeds as follows. Let $\boldsymbol{\xi} = \nabla V/\|\nabla V\|$ be the unit normal vector to Σ_v at a given point x, and let $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ be any basis for the tangent space of Σ_v at x. Then [11]

$$K_G(x) = \frac{(-1)^n}{\|\nabla V\|^n} \left| \begin{pmatrix} \nabla_{\mathbf{v}_1}\nabla V \\ \vdots \\ \nabla_{\mathbf{v}_n}\nabla V \\ \nabla V \end{pmatrix} \right| \left| \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_n \\ \nabla V \end{pmatrix} \right|^{-1} . \quad (6)$$

Let us now consider the family of $\{\Sigma_v\}_{v\in\mathbb{R}}$ associated with a particular physical system and show how things work in practice. We consider the so-called φ^4 model on a d-dimensional lattice $\mathbb{Z}^d$ with $d = 1, 2$, described by the potential function

$$V = \sum_{i\in\mathbb{Z}^d} \left(-\frac{\mu^2}{2} q_i^2 + \frac{\lambda}{4} q_i^4 \right) + \sum_{\langle ik\rangle\in\mathbb{Z}^d} \frac{1}{2} J(q_i - q_k)^2 , \quad (7)$$

where $\langle ik\rangle$ stands for nearest-neighbor sites. This system has a discrete $\mathbb{Z}_2$ symmetry and short-range interactions; therefore, according to the Mermin-Wagner theorem, in $d = 1$ there is no phase transition whereas in $d = 2$ there is a symmetry-breaking transition of the same universality class of the 2D Ising model.

Independently of any statistical measure, let us now probe, by computing $\chi(\Sigma_v)$ vs v according to Eq. (5), if and how the topology of the hypersurfaces Σ_v varies with v. To this aim we first devised an algorithm of Monte Carlo type by constructing a Markov chain on any desired surface Σ_v. This is obtained by means of a “demon” algorithm corrected with a projection technique [12] which provides a simple and efficient method to constrain a random walk on a level hypersurface, here, of the potential function. Each new step so obtained on Σ_v

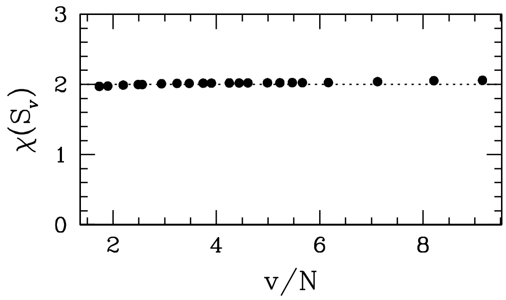

FIG. 1. Numerical computation of the Euler characteristic for 24-dimensional spheres. v is the squared radius.

represents a trial step which is accepted or rejected according to a Metropolis-like "importance sampling" criterion [13] adapted to the weight $\sqrt{\det(g)}$. With any Monte Carlo scheme we can actually compute densities, that is we can estimate only $\int_{\Sigma_v} K_G \, d\sigma / \int_{\Sigma_v} d\sigma$, the average of K_G, rather than its total value (5) on Σ_v, hence the need for an estimate of $\mathrm{Area}(\Sigma_v) = \int_{\Sigma_v} d\sigma$ as a function of v. To this aim we worked out a geometric formula that links the relative variation of $\mathrm{Area}(\Sigma_v)$ with respect to an arbitrary initial value $\mathrm{Area}(\Sigma_{v_0})$, to another Monte Carlo average on Σ_v: $\langle M_1 / \|\nabla V\| \rangle_{MC}^{\Sigma_v}$ where $M_1 = \frac{1}{n} \sum_{i=1}^{n} \kappa_i$ is the mean curvature of Σ_v [14]. Thus the final outcomes of our computations are the *relative* variations of the Euler characteristic. The computation of K_G at any point $x \in \Sigma_v$ proceeds by working out an orthogonal basis for the tangent space at x, orthogonal to $\boldsymbol{\xi} = \nabla V / \|\nabla V\|$, by means of a Gram-Schmidt orthogonalization procedure. Then Eq. (6) is used to compute K_G at x. On each Σ_v we sampled 1×10^6–3.5×10^6 points where we computed K_G. This number of points was varied, and several initial conditions were also considered in order to check the stability of the results. The computations were performed for $\dim(\Sigma_v) = 48, 80$ (i.e., $N = 7 \times 7, 9 \times 9$) and with the choice $\lambda = 0.6, \mu^2 = 2, J = 1$ for the parameters of the potential. In order to test the correctness of our numerical "protocol" to compute $\chi(\Sigma_v)$, and to assess its degree of reliability, we checked the method against a simplified form of the potential V in Eq. (7), i.e., with $\lambda = J = 0, \mu^2 = -1$. In this case the Σ_v are hyperspheres and therefore $\chi(\mathbb{S}_v^n) = 2$ for any even n. $\mathrm{Area}(\mathbb{S}_v^n)$ is analytically known as a function of the radius $\sqrt{v}$, therefore the starting value $\mathrm{Area}(\Sigma_{v_0})$ is known, and in this case we can compute the actual values of $\chi(\Sigma_v)$ instead of their relative variations only.

In Fig. 1 we report $\chi(\Sigma_v = \mathbb{S}_v^n)$ vs v/N for $N = 5 \times 5$; the results are in agreement with the theoretical value within an error of a few percent, a very good precision in view of the large variations of $\chi(\Sigma_v)$ that are found with the full expression (7) of V. In Fig. 2 we report the results for the 1D lattice, which is known to not undergo any phase transition. Apart from some numerical noise—here enhanced by the more complicated topology

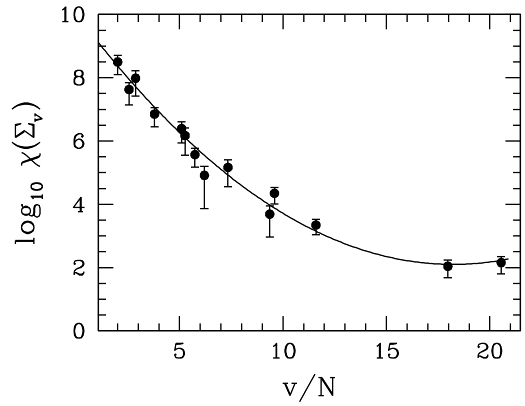

FIG. 2. 1D φ^4 model. Relative variations of the Euler characteristic of Σ_v vs v/N (potential energy density). Lattice of $N = 1 \times 49$ sites. Full line is a guide to the eye.

of the Σ_v when $\lambda, J \neq 0$—a monotonously (in the average) decreasing pattern of $\chi(v/N)$ is found. Since the variation of $\chi(v/N)$ signals a topology change of the $\{\Sigma_v\}$, Fig. 2 tells that a "smoothly" varying topology is not *sufficient* for the appearance of a phase transition. In fact, when the 2D lattice is considered, the pattern of $\chi(v/N)$ is very different: it displays a rather abrupt *change of the topology variation rate with* v/N at some v_c/N. This result is reported in Fig. 3 for a lattice of $N = 7 \times 7$ sites, and in Fig. 4 for a larger lattice of $N = 9 \times 9$ sites [15].

The question is now whether the value v_c/N, at which $\chi(v/N)$ displays a cusp, has anything to do with the thermodynamic phase transition, i.e., we wonder if the effective support of the canonical measure shrinks close to $\Sigma_{v \equiv v_c}$ just at $\beta \equiv 1/T_c$, the (inverse) critical temperature of the phase transition. The answer is in the affirmative. In fact, the numerical analysis in Refs. [4,16] shows that—with $\lambda = 0.6, \mu^2 = 2, J = 1$—the function

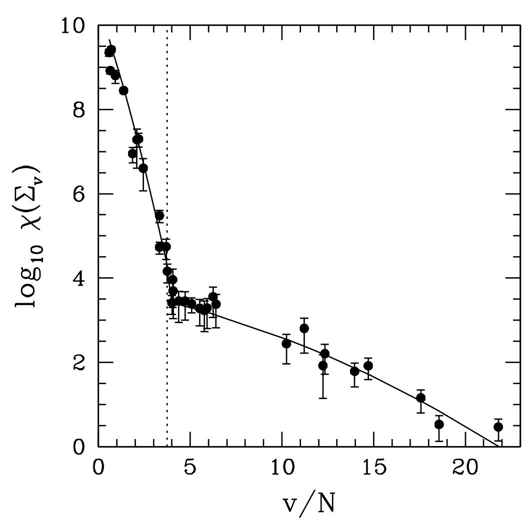

FIG. 3. 2D φ^4 model. Relative variations of the Euler characteristic of Σ_v vs v/N (potential energy density). Lattice of $N = 7 \times 7$ sites. The vertical dotted line corresponds to the phase transition point. Full line is a guide to the eye.

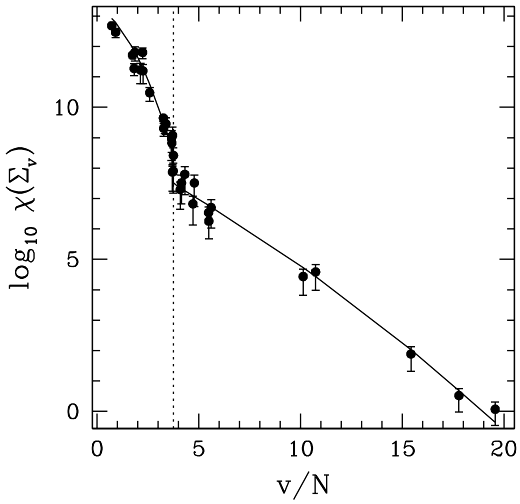

FIG. 4. 2D φ^4 model. Relative variations of the Euler characteristic of Σ_v vs v/N (potential energy density). Lattice of $N = 9 \times 9$ sites. The vertical dotted line corresponds to the phase transition point. Full line is a guide to the eye.

$\frac{1}{N}\langle V\rangle(T)$ and its derivative signal the phase transition at $\frac{1}{N}\langle V\rangle \simeq 3.75$, a value in very good agreement—within the numerical precision—with v_c/N where the cusp of $\chi(v/N)$ shows up. Through the computation of the v dependence of a topologic invariant, the hypothesis of a deep connection between topology changes of the $\{\Sigma_v\}$ and phase transitions has been given a direct confirmation. Moreover, we found that a sudden *second order variation* of the topology of these hypersurfaces is the "suitable" topology change—mentioned at the beginning of the present Letter—that underlies the phase transition of second kind in the lattice φ^4 model.

There is no reason why the results presented here should be peculiar only to the chosen model, and therefore they point to a general validity of the relationship between topology and phase transitions, opening a wide field of future investigations and applications.

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[14] $\mathrm{Area}(\Sigma_v) = \mathrm{Area}(\Sigma_{v_0}) \exp \int_{v_0}^{v} du\, \langle M_1/\|\nabla V\|\rangle_{MC}^{\Sigma_u}$ is the formula we used. It stems from $\psi(v) = \log \mathrm{Area}(\Sigma_v)$ and the quadrature of $\psi'(v) = [d/dv\, \mathrm{Area}(\Sigma_v)]/\mathrm{Area}(\Sigma_v)$ written using a geometric derivation formula in Ref. [2].

[15] We could not perform a systematic study of finite-size effects, beyond this check with two different lattice sizes, for two reasons: (i) the computation of $\chi(v/N)$ is very heavy (the results reported here required more than 6000 CPU hours on fast hp workstations); (ii) $\chi(v/N)$ is not a thermodynamic observable, and in fact it is neither an intensive nor an extensive quantity, moreover, according to the form of the potential, its dependence upon the dimension of the Σ_v can be of any kind; there are manifolds whose Betti numbers (in terms of which χ is defined) are factorially growing with N, others—like hyperspheres—for which χ is a constant independent of N.

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