Topology and phase transitions: From an exactly solvable model to a relation between topology and thermodynamics

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The elsewhere surmized topological origin of phase transitions is given here important evidence through the analytic study of an exactly solvable model for which both topology of submanifolds of configuration space and thermodynamics are worked out. The model is a mean-field one with a k-body interaction. It undergoes a second-order phase transition for $k=2$ and a first-order one for $k>2$. This opens a perspective for the understanding of the deep origin of first and second-order phase transitions, respectively. In particular, a remarkable theoretical result consists of a mathematical characterization of first-order transitions. Moreover, we show that a "reduced" configuration space can be defined in terms of collective variables, such that the correspondence between phase transitions and topology changes becomes one-to-one, for this model. Finally, an unusual relationship is worked out between the microscopic description of a classical N-body system and its macroscopic thermodynamic behavior. This consists of a functional dependence of thermodynamic entropy upon the Morse indexes of the critical points (saddles) of the constant energy hypersurfaces of the microscopic $2N$-dimensional phase space. Thus phase space (and configuration space) topology is directly related to thermodynamics.

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I. INTRODUCTION

Thermodynamical phase transitions are certainly one of the main topics of statistical physics. A huge amount of work, both theoretical and experimental, has been done during the past decades leading to remarkable successes as is witnessed, for example, by the renormalization group theory of critical phenomena. However, there are still long-standing open problems about phase transitions; among them we can mention amorphous and disordered systems (like glasses and spin glasses) undergoing "dynamical" transitions, or first-order phase transitions, which are still lacking a satisfactory theoretical understanding of their origin. Moreover, on the forefront of modern research in statistical physics, standard theoretical definitions and methods are challenged by the experimentally observed phase transitions occurring in small classical and quantum systems (nanoscopic and mesoscopic) like atomic and molecular clusters, polymers and proteins, Bose-Einstein condensates, droplets of quantum liquids, etc. Finally, in the mathematically rigorous background of phase transitions theory, neither in the Yang-Lee theory for the grand canonical ensemble [1] nor in the Ruelle, Sinai, Pirogov theory for the canonical ensemble [2], an *a priori* mathematical distinction can be made among the potentials leading to first or second-order phase transitions, respectively.

The present paper aims to contribute to the advancement of a recently proposed theoretical framework where the singular behaviors of thermodynamic observables at a phase transition are attributed to major topology changes in phase space and—equivalently—in configuration space [3–7]. More precisely, in Refs. [3–7], it has been proposed that thermodynamic phase transitions could be a consequence of suitable topology changes of certain submanifolds of the configuration space defined by the potential energy function. The presence of such topological changes has been recently shown to be a *necessary* condition, under fairly general assumptions, for the presence of a phase transition [8]; however, the converse is *not* true, and no rigorous results are available yet on the sufficient conditions. The analytical or numerical study of particular models thus remains crucial to get hints towards more general results (see also Refs. [9,10] for recent results on one-dimensional systems, and Ref. [11] as to the fully connected spherical model).

In this perspective, we stress that the topological approach has been hitherto applied only to systems undergoing

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second-order phase transitions. Therefore tackling first-order phase transitions in the topological framework is of great interest, because some insight into the challenging problem of their origin can be obtained, and because this reinforces the working hypothesis that the topological approach could unify the treatment of the different kinds of phase transitions in view of encompassing also more "exotic" ones, like glassy transitions and the others mentioned earlier.

In this paper we first study a model which, according to the value of a parameter, has no transition or undergoes a first or a second-order transition. Remarkably, for this model an exact analytical computation is possible of the Euler characteristic—that is a topological invariant—of those submanifolds of the configuration space whose topological changes are expected to be related to the phase transition. We find [12] that the phase transition is actually signaled by a discontinuity in the Euler characteristic $\chi(e)$ and that the sign of the second derivative of $\chi(e)$ indicates the order of the transition. Then, we study the topology of submanifolds of a "reduced" configuration space, i.e., the space of some collective variables: in this case we find a one-to-one correspondence between phase transitions and topology changes.

Finally, we derive a general result showing that an analytic *estimate* of another topological invariant of the same submanifolds can be worked out which allows to directly link topology and thermodynamic entropy.

II. A KEY STUDY

In this section we present a study of the thermodynamical properties of the mean-field k-trigonometric model (kTM), as well as of the topological properties of its configuration space. A preliminary study of this model along these lines has already been reported in Ref. [12]; there only the microcanonical thermodynamics was considered, while here we are going to discuss also the canonical thermodynamical properties. Being a model with long-range interactions which may undergo also first-order phase transitions, we expect canonical and microcanonical thermodynamic functions to be different, at least close to first-order transitions [13].

The kTM is defined by the Hamiltonian

$$H_k = \sum_{i=1}^{N} \frac{1}{2}\pi_i^2 + V_k(\varphi_1, \ldots, \varphi_N), \tag{1}$$

where $\{\varphi_i\}$ are angular variables: $\varphi_i \in [0, 2\pi)$, $\{\pi_i\}$ are the conjugated momenta, and the potential energy V is given by

$$V_k = \frac{\Delta}{N^{k-1}} \sum_{i_1,\ldots,i_k} [1 - \cos(\varphi_{i_1} + \cdots + \varphi_{i_k})], \tag{2}$$

where Δ is the coupling constant. In what follows only the potential energy part will be considered. This interaction energy is apparently of a mean-field nature, in that each degree of freedom interacts with all the others; moreover, the interactions are k-body ones.

The kTM is a generalization of the trigonometric model (TM) introduced by Madan and Keyes [14] as a simple model for the potential energy surface (PES)—the hypersurface defined by the potential energy as a function of the N degrees of freedom—of simple liquids. The TM is a model for N independent degrees of freedom with potential energy (2) with $k=1$: $V_{k=1}$.

It shares with Lennard-Jones-like systems [15] the existence of a regular organization of the critical points of the potential energy above a given minimum (the elevation in energy of the critical points is proportional to their index) and a regular distribution of the minima in the configuration space (nearest-neighbor minima lie at a well defined Euclidean distance). The PES of the kTM maintains the main features of the TM [16], introducing, however, a more realistic feature, namely the interaction among the degrees of freedom (in the form of a k-body interaction).

Using the relation

$$\cos(\varphi_{i_1} + \cdots + \varphi_{i_k}) = \mathrm{Re}(e^{i\varphi_{i_1}} \cdots e^{i\varphi_{i_k}}), \tag{3}$$

the configurational part of the Hamiltonian can be written as

$$V_k = N\Delta[1 - \mathrm{Re}\ (c + is)^k] = N\Delta\left[1 - \sum_{n=0}^{[k/2]} \binom{k}{2n} \times (-1)^n c^{k-2n} s^{2n}\right], \tag{4}$$

where c and s are collective variables, functions of $\{\varphi_i\}$:

$$c = \frac{1}{N}\sum_i \cos\ \varphi_i,$$

$$s = \frac{1}{N}\sum_i \sin\ \varphi_i. \tag{5}$$

We observe also that the model has a symmetry group obtained by the transformations

$$\varphi_i \to \varphi_i + \ell\frac{2\pi}{k},$$

$$\varphi_i \to -\varphi_i. \tag{6}$$

If we think of φ_i as the angle between a unitary vector in a plane and the horizontal axis of this plane, we find that the first transformations are rotations in this plane of an angle $\ell(2\pi/k)$ and the second is the reflection with respect to the horizontal axis. This group is also called C_{kv}.

Let us now derive the thermodynamical properties of the kTM.

A. Canonical thermodynamics

The partition function is

$$Z_k = \int d\{\varphi\} e^{-\beta H_k} = \int d\{\varphi\} e^{-\beta N\Delta[1-\mathrm{Re}(c+is)^k]}, \tag{7}$$

introducing δ functions for the variables c and s:

$$Z_k = \int d\{\varphi\} \int dx\, dy\, \delta(x-c)\,\delta(y-s) e^{-\beta N \Delta [1-\mathrm{Re}(x+iy)^k]}, \tag{8}$$

and using the integral representation of the δ function, we obtain for Z_k:

$$\begin{aligned} Z_k &= \int d\{\varphi\} \int dx\, dy \int N^2 \frac{d\lambda}{2\pi}\frac{d\mu}{2\pi} \\ &\quad \times e^{iN\lambda(x-c)} e^{iN\mu(y-s)} e^{-\beta\Delta N[1-\mathrm{Re}(x+iy)^k]} \\ &= \int dx dy e^{-\beta\Delta N[1-\mathrm{Re}\ (x+iy)^k]} \\ &\quad \times \int N^2 \frac{d\lambda}{2\pi}\frac{d\mu}{2\pi} e^{iN(\lambda x+\mu y)} \\ &\quad \times \int d\{\varphi\} e^{-iN(\lambda c+\mu s)}. \end{aligned} \tag{9}$$

The last integral is easily computable using Eq. (5):

$$\int d\{\varphi\} e^{-iN(\lambda c+\mu s)} = \left[\int_0^{2\pi} d\varphi e^{-i(\lambda\ \cos\ \varphi+\mu\ \sin\ \varphi)} \right]^N, \tag{10}$$

and can be written in term of the Bessel function J_0:

$$\int_0^{2\pi} d\varphi e^{-i\Lambda\ \cos(\varphi-\psi)} = 2\pi J_0(\Lambda), \tag{11}$$

where $\lambda = \Lambda \cos\psi$, $\mu = \Lambda \sin\psi$, and $\Lambda = \sqrt{\lambda^2+\mu^2}$. The partition function can then be written as

$$\begin{aligned} Z_k &= N^2 (2\pi)^{N-2} \int dx dy d\lambda d\mu \\ &\quad \times e^{-N[-i\lambda x - i\mu y + \beta\Delta - \beta\Delta \mathrm{Re}(x+iy)^k - \log(J_0(\Lambda))]}, \end{aligned} \tag{12}$$

and since the J_0 function is always positive, there are no problems in defining its logarithm.

We want now to perform a saddle-point evaluation of the integral, so we have to look for the minima of the exponent in the complex λ, μ, x, y plane. We note that if that points do not lie on the imaginary axis of the λ, μ planes, the free energy of the model would be imaginary. So we can safely rotate the integration path on the imaginary axis in the λ, μ planes, which corresponds to the substitutions: $i\lambda \to \lambda$ and $i\mu \to \mu$, then $i\Lambda \to \Lambda$ and $J_0(\Lambda) \to I_0(\Lambda)$, where I_0 is the modified Bessel function

$$I_0(\Lambda) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{\Lambda\ \cos\ \varphi}. \tag{13}$$

In conclusion we obtain

$$Z_k = N^2 (2\pi)^{N-2} \int dx dy d\lambda d\mu e^{-N g_k(x,y,\lambda,\mu;\beta)}, \tag{14}$$

where g_k is the real function

$$\begin{aligned} g_k(x,y,\lambda,\mu;\beta) &= \beta\Delta - \lambda x - \mu y - \beta\Delta\ \mathrm{Re}(x+iy)^k \\ &\quad - \log[I_0(\Lambda)]. \end{aligned} \tag{15}$$

In order to find the stationary points, we first determine the subspace defined by the equations

$$\frac{\partial g_k}{\partial x} = 0, \tag{16}$$

$$\frac{\partial g_k}{\partial y} = 0, \tag{17}$$

obtaining the relations

$$\lambda = -\beta\Delta k\ \mathrm{Re}(x+iy)^{k-1}, \tag{18}$$

$$\mu = \beta\Delta k\ \mathrm{Im}(x+iy)^{k-1}, \tag{19}$$

thus we get

$$\Lambda = \beta\Delta k |(x+iy)^{k-1}|. \tag{20}$$

Now, using Eqs. (18) and (19), we can substitute λ and μ with x and y in Eq. (15), obtaining, in term of the complex number $z = x+iy$:

$$g_k(z;\beta) = \beta\Delta + \beta\Delta(k-1)\mathrm{Re}\ z^k - \log\ I_0(\beta\Delta p |k^{p-1}|), \tag{21}$$

and using the polar representation $z = \rho e^{i\psi}$:

$$g_k(\rho,\psi;\beta) = \beta\Delta + \beta\Delta(k-1)\rho^k \cos(k\psi) - \log\ I_0(\beta\Delta k \rho^{k-1}). \tag{22}$$

The derivative with respect to ψ leads to

$$-\beta\Delta(k-1)k\rho^k \sin(k\psi) = 0, \tag{23}$$

so that there are $2k$ solutions

$$\psi_n = \frac{n\pi}{k} (n = 1, \ldots, 2k). \tag{24}$$

Observing that $\cos(k\psi_n) = (-1)^n$ we obtain

$$g_k(\rho,n;\beta) = \beta\Delta + (-1)^n \beta\Delta(k-1)\rho^k - \log\ I_0(\beta\Delta k \rho^{k-1}) \tag{25}$$

and we can restrict ourselves to $n = 0, 1$. Finally, the derivative with respect to ρ leads to the stationary points equation

$$(-1)^n \rho = \frac{I_1(\beta\Delta k \rho^{k-1})}{I_0(\beta\Delta k \rho^{k-1})}, \tag{26}$$

where the modified Bessel function I_1 is defined by

$$I_1(\Lambda) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi\ \cos\ \varphi e^{\Lambda\ \cos\ \varphi} = I_0'(\Lambda). \tag{27}$$

For $n = 1$ we have only the trivial solution $\rho = 0$, because the I functions are always positive. By using an expansion for small ρ one can show that this solution is a maximum for g. So we can study only the case $n = 0$. We note that if there is a nontrivial solution (i.e., $\tilde{\rho}(\beta) \neq 0$) of Eq. (26), calling $\tilde{g}_k(\beta)$ the value of $g_k[\beta, \tilde{\rho}(\beta)]$, we have

$$Z_k \sim N^2(2\pi)^{N-2}e^{-N\tilde{g}_k(\beta)}, \tag{28}$$

and the free energy and internal energy are, respectively,

$$f_k(\beta) = \beta^{-1}\tilde{g}_k(\beta) - \beta^{-1}\log(2\pi), \tag{29}$$

$$e_k(\beta) = \Delta(1-\tilde{\rho}^k). \tag{30}$$

Let us now analyze the case $k=1$. In this case the solutions $\rho=0$ are not present, so that we have only the solution

$$\tilde{\rho} = \frac{I_1(\beta\Delta)}{I_0(\beta\Delta)}. \tag{31}$$

There is no phase transition, and using Eq. (30) we have

$$e_1(\beta) = \Delta\left[1 - \frac{I_1(\beta\Delta)}{I_0(\beta\Delta)}\right]. \tag{32}$$

This is the free energy of trigonometric model that has been mentioned before.

For $k=2$ the solution $\rho=0$ is stable for high temperatures, but a nontrivial solution of Eq. (26) appears at $\beta\Delta=1$. The transition temperature is given by the condition

$$\left.\frac{d^2g_2(\rho;\beta_c)}{d\rho^2}\right|_{\rho=0} = 2\beta_c\Delta(1-\beta_c\Delta) = 0, \tag{33}$$

so that we obtain $\beta_c\Delta=1$; the transition is continuous, and the order parameter is $\tilde{\rho}$. It is easy to show that $\tilde{x}=\langle c\rangle$ and $\tilde{y}=\langle s\rangle$ [e.g., by adding an external field of the form $-N(hc+ks)$ to the Hamiltonian and performing the limit $h,k\to 0$]; then the vector $(\tilde{x},\tilde{y})$ is the mean magnetization of the spins represented by the φ_i. As $\tilde{\rho}$ is the modulus of the magnetization, for $\beta\Delta>1$, when $\tilde{\rho}\neq 0$, the C_{2v} symmetry is broken.

When $k>2$, the nontrivial solution of Eq. (26) appears at a given β' but becomes stable only at $\beta''>\beta'$, so that $\tilde{\rho}(\beta)$ and $e(\beta)$ are discontinuous at β''; instead of the instability region $\beta'<\beta<\beta''$, in the microcanonical ensemble a region where the specific heat is negative appears, as we shall see later. The C_{kv} symmetry is broken in the low temperature phase, so that $\tilde{\rho}$ can be used as an order parameter in revealing the symmetry breaking, even if it is not continuous at β''. The transition is then of first order, but keeps the symmetry structure of a second order one, i.e., in the low temperature phase there are k pure states related by the symmetry group also in the case of the first order transition.

In Fig. 1 we report the caloric curve, i.e., the temperature $T=\beta^{-1}$ as a function of the average energy (per degree of freedom) e, for three values of k, $k=1$, 2, and 3. As previously discussed, the temperature is an analytic function of e for $k=1$; for $k=2$ the system undergoes a second order phase transition at a critical temperature $T_c=\Delta$, that changes to first order for $k>2$.

In Figs. 2 and 3 we report the average potential energy v as a function of the average energy e and the temperature T as a function of v, respectively. It is apparent that, for $k\geqslant 2$, the phase transition point always corresponds to $v_c=\Delta$.

Another feature which shows up in Figs. 2 and 3 is that the average potential energy v never exceeds the value Δ, i.e., although the maximum of V/N is equal to 2Δ, the region $v>\Delta$ is not thermodynamically accessible to the system. The

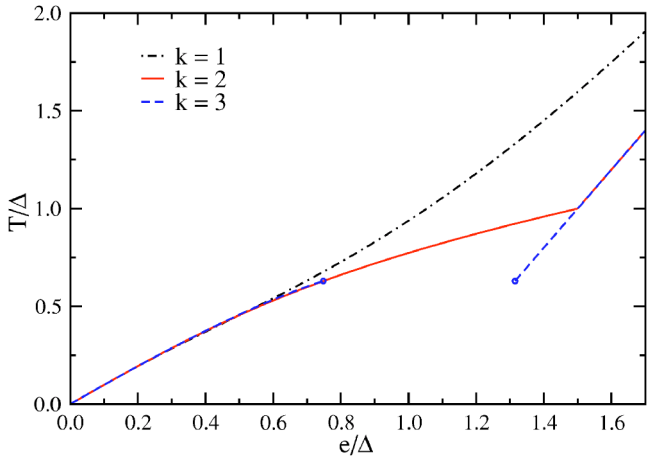

FIG. 1. Temperature T as a function of canonical average energy e for three different values of k; for $k=1$ there is no phase transition, while for $k=2$ there is a second order transition and for $k>2$ a first order one.

reason for this is in the mean-field nature of the system and in the fact that we are working in the thermodynamic limit $N\to\infty$. According to Eqs. (4), the potential energy can be written as a function of the collective variables c and s defined in Eqs. (5), which are the components of the function whose statistical average is the order parameter, i.e., the "magnetization." In the thermodynamic limit these functions become constants, whose value coincides with their statistical average, and since $\langle c\rangle=\langle s\rangle=0$ for $T>T_c$, and from Eqs. (4) this implies $v=\Delta$ for all $T>T_c$.

As we shall see later, this fact remains true also in the microcanonical ensemble, which, however, is *not* equivalent to the canonical ensemble for the present model, due to the long-range nature of the interactions.

B. Microcanonical thermodynamics

As in other simple mean-field models, also in the case of the kTM it is possibile to perform a calculation of the micro-

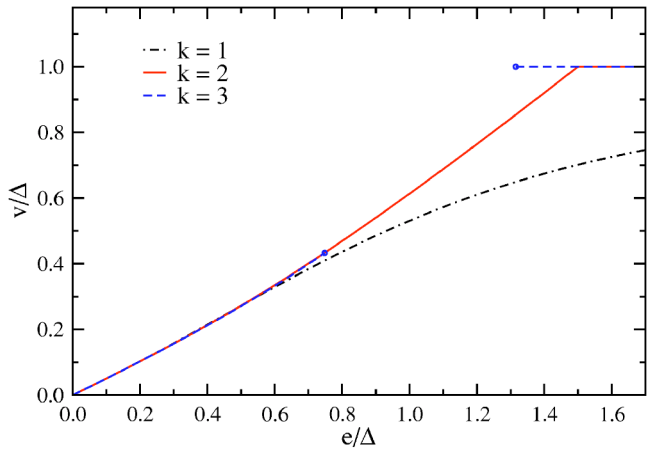

FIG. 2. Canonical average potential energy v as a function of canonical average energy e for $k=1$, 2 and 3. The upper phase transition point is, for $\forall k\geqslant 2$, $v_c=\Delta$.

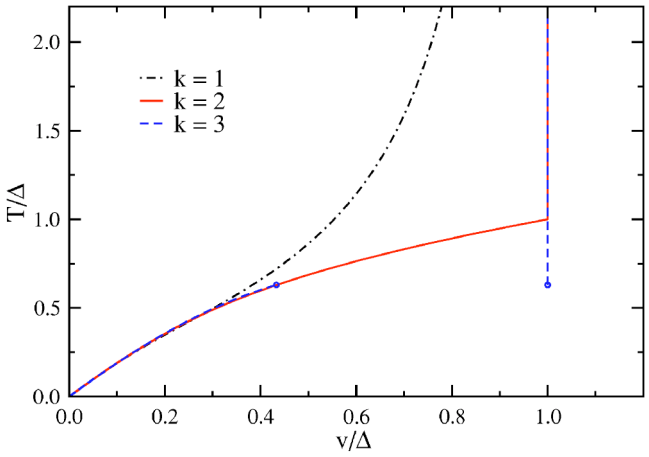

FIG. 3. Temperature T as a function of canonical average potential energy v for three different values of k.

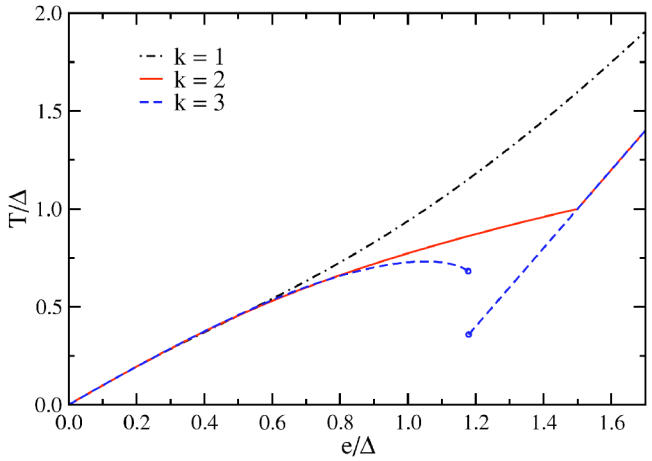

FIG. 4. Microcanonical temperature T as a function of energy e for three different values of k; for $k=1$ there is no phase transition, while for $k=2$ there is a second order transition and for $k>2$ a first order one.

canonical partition function, or microcanonical density of states in phase space, given by

$$\Omega_{N,k}(E) = \int \frac{d^N \pi d^N \varphi}{N!} \delta(H_k - E). \tag{34}$$

The computation of Ω is similar to that of Z in the canonical case, so that we will go through it with less detail.

Using the integral representation of the delta function, we get

$$\Omega_{N,k}(E) = \int \frac{d\beta}{2\pi} \int \frac{d^N \pi d^N \varphi}{N!} e^{-i\beta(H_k - E)}. \tag{35}$$

Now, as we are looking for a saddle-point evaluation of the integral over β, we can rotate the integration path on the imaginary axis in the complex- β plane. This is justified because, as in the canonical case, the saddle point is located on this axis. We can now perform the integration over the momenta and use the fact that $V_k(\varphi) = V_k[c(\varphi), s(\varphi)]$, see Eq. (4), to obtain

$$\Omega_{N,k}(E) = \mathcal{C}_N \rho^N \int d\beta d\xi d\eta \beta^{-\frac{N}{2}} e^{\beta[E - V_k(\xi,\eta)]} \times \int d^N \varphi \delta\{N[\xi - c(\varphi)]\} \delta\{N[\eta - s(\varphi)]\}, \tag{36}$$

where $\rho = N/L$ and the constant $\mathcal{C}_N$ gives only a constant contribution to the entropy per particle, i.e., it is at most of order e^N. The last integral can be evaluated using again the integral representation of the delta function, and rotating then the integration path as previously discussed; it turns out to be

$$\int \frac{d\mu\, d\nu}{(2\pi)^2} e^{-N(\mu\xi + \nu\eta)} \int d^N \varphi e^{\Sigma_i (\mu \cos \varphi_i + \nu \sin \varphi_i)} = \int \frac{d\mu d\nu}{(2\pi)^2} e^{-N(\mu\xi + \nu\eta)} [2\pi I_0(\Lambda)]^N,$$

having defined $\Lambda = \sqrt{\mu^2 + \nu^2}$; I_0 is a Bessel function as before. We can then write the density of states as

$$\Omega_{N,k}(e) = \mathcal{C}_N \rho^N \int d\mathbf{m} e^{N f_k(\mathbf{m},e)}, \tag{37}$$

where $\mathbf{m} \equiv (\beta, \xi, \eta, \mu, \nu)$, $e = E/N$ and

$$f_k(\mathbf{m},e) = \beta e - \beta\Delta[1 - \mathrm{Re}(\xi + i\eta)^k] - \tfrac{1}{2}\log \beta - \mu\xi - \nu\eta + \log I_0(\Lambda).$$

Then, using the saddle-point theorem, the entropy per particle, $s = S/N$, is given by ($k_B = 1$):

$$s_k(e) = \lim_{N\to\infty} \frac{1}{N} \log \Omega_{N,k}(e) = \max_{\mathbf{m}} f_k(\mathbf{m},e). \tag{38}$$

To find the maximum of $f_k(\mathbf{m},e)$ one can calculate analytically some derivatives of f to obtain a one-dimensional problem that can be easily solved numerically with standard methods.

As already done in the case of the canonical ensemble, in Fig. 4 we report the microcanonical caloric curve, i.e., the temperature T as a function of the energy (per degree of freedom) e, $T(e) = [\partial s/\partial e]^{-1}$ for three values of k, $k=1$, 2, and 3. As in the canonical case, the temperature is an analytic function of e for $k=1$, while for $k=2$ the system undergoes a second-order phase transition at a certain energy value e_c, that changes to first order for $k>2$.

We note that, for $k>2$, in a region of energies smaller than the critical energy e_c of the first-order phase transition the curve $T(e)$ has a negative slope, i.e., the system has a negative specific heat. The kTM is then another physical model where this feature is found (see, e.g., Ref. [13] for other examples). This is not surprising at all since we are considering the *microcanical* thermodynamics of a system with long-range interactions; such a region is *not* present when we consider the canonical ensemble, as shown earlier; there, the region of negative specific heat corresponds to the region of instability of the non-trivial solution of the saddle-point equations.

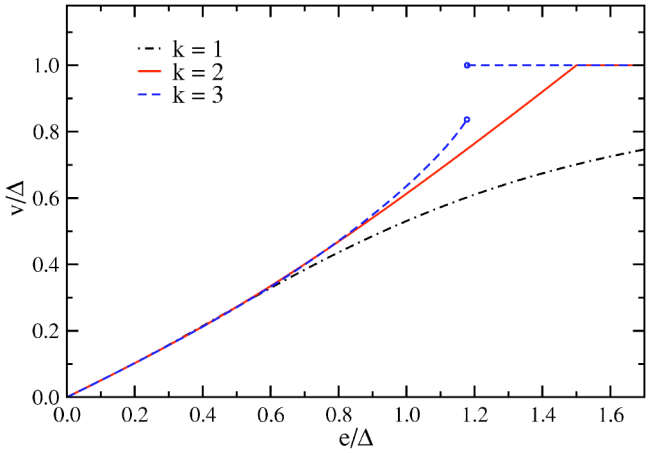

FIG. 5. Microcanonical average potential energy v as a function of energy e for $k=1,2$, and 3. The phase transition point is, for $\forall k \geqslant 2$, $v_c=\Delta$.

In Figs. 5 and 6 we report the average microcanonical potential energy v as a function of e and the microcanonical temperature T as a function of v, respectively. It is apparent that, for $k \geqslant 2$, the phase transition point always corresponds to $v_c=\Delta$.

As in the canonical case, the average potential energy v never exceeds the value Δ, i.e., the region $v>\Delta$ is not thermodynamically accessible to the system also in the microcanonical ensemble.

C. Topology of configuration space

In this section we want to investigate the relation between the phase transitions occurring in the kTM and the topology of its configuration space. Given the potential energy V, the following submanifolds of configuration space are defined:

$$M_v \equiv \{\varphi | V(\varphi) \leqslant Nv\}.$$

As v varies from the minimum to the maximum allowed value of $V(\varphi)/N$, the manifolds M_v progressively cover the whole configuration space. These submanifolds, or their boundaries $\Sigma_v=\partial M_v$, are then a possible way to depict the potential energy landscape of the system. The topology of the M_v's can be studied using Morse theory [17]: whenever a *critical value* of $V(\varphi)/N$—i.e., a value corresponding to one or more *critical points*, where the differential of $V(\varphi)/N$ vanishes—is crossed, the topology of the M_v's change. It has been conjectured [3,6] that some of these topology changes are the "deep" cause of the presence of a phase transition. The correspondence between major topology changes of the M_v's and Σ_v's and phase transitions has been checked in two particular models [5,7]; more recently, it has been proved [8] that a topology change is a *necessary* condition for a phase transition under rather general assumptions [28], but the sufficiency conditions are still lacking.

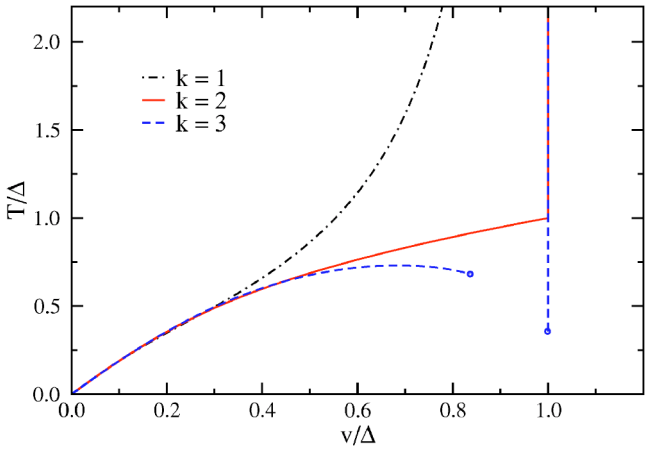

FIG. 6. Microcanonical temperature T as a function of microcanonical average potential energy energy v for three different values of k.

A natural way to characterize topology changes involves the computation of some *topological invariants* of the manifolds under investigation. One of such invariants is the Euler characteristic χ: in Refs. [5,7] it was shown that the Euler characteristic $\chi(v)$ of the submanifolds M_v and/or of the Σ_v shows a singularity in correspondence of the potential energy value $v_c=v(e_c)$ at which the transition takes place: this seems then to signal a particularly "strong" topology change. Remarkably, the Euler characteristic of M_v can be calculated *analytically* in our model. The general definition is [18]:

$$\chi(v) \equiv \chi(M_v) = \sum_{i=0}^{N} (-1)^i \mu_i(M_v), \tag{39}$$

where the *Morse numbers* $\mu_i(M_v)$ are the number of critical points of index i of the function $V(\varphi)$ that belong to the manifold M_v. As already mentioned, the critical points (called *saddles* in other contexts, e.g., in the physics of glasses) $\tilde{\varphi}$ are defined by the condition $dV_k(\tilde{\varphi})=0$, and their index i (otherwise called the *order* of the saddle) is defined as the number of negative eigenvalues of the Hessian matrix

$$\mathcal{H}_{ij}^k(\tilde{\varphi}) = \left(\frac{\partial^2 V_k}{\partial \varphi_i \, \partial \varphi_j} \right) \Bigg|_{\tilde{\varphi}}. \tag{40}$$

To be valid, Eq. (39) requires that $V(\varphi)$ is a Morse function, i.e., that its critical points are nondegenerate: this means that all the eigenvalues of the Hessian are nonzero at a critical point and that the critical points themselves are isolated.

To determine the critical points we have then to solve the system

$$\frac{\partial V_k}{\partial \varphi_j} = 0 \qquad \forall \, j = 1, \ldots, N \tag{41}$$

that is, inserting Eq. (4) in the earlier equations

$$-\Delta k \, \mathrm{Re}[i(c+is)^{k-1} e^{i\varphi_j}] = \Delta k \zeta^{k-1} \sin[(k-1)\psi + \varphi_j] = 0$$
$$\forall \, j = 1, \ldots, N, \tag{42}$$

where we defined $c+is=\zeta e^{i\psi}$. From Eq. (4) we have

$$V_k(\varphi) = N\Delta[1 - \zeta^k \cos(k\psi)], \tag{43}$$

then all the critical points with $\zeta(\tilde{\varphi})=0$ have energy $v=V(\tilde{\varphi})/N=\Delta$. We note that they correspond to vanishing

magnetization. Let us now consider all the critical points with $\zeta(\tilde{\varphi}) \neq 0$. Then Eq. (42) becomes

$$\sin[(k-1)\psi + \varphi_j] = 0,$$

$$\forall j = 1, \ldots, N, \tag{44}$$

and its solutions are

$$\tilde{\varphi}_j^{\mathbf{m}} = [m_j \pi - (k-1)\psi]_{\mathrm{mod}\ 2\pi}, \tag{45}$$

where $m_j \in \{0,1\}$. Since in Eq. (42) ζ appears to the $k-1$th power, in the case $k=1$ Eqs. (42) and (44) coincide. This means that the solutions given in Eq. (45) are *all* the critical points, regardless of their energy, in the case $k=1$ and all the critical points *but* those with energy $v=\Delta$ in the case $k>1$. The critical point $\tilde{\varphi}^{\mathbf{m}}$ is then characterized by the set $\mathbf{m} \equiv \{m_j\}$. To determine the unknown constant ψ we have to substitute Eq. (45) in the self-consistency equation

$$\zeta e^{i\psi} = c + is = N^{-1} \sum_j e^{i\varphi_j} = N^{-1} e^{-i\psi(k-1)} \sum_j (-1)^{n_j}. \tag{46}$$

If we introduce the quantity $n(\tilde{\varphi})$ defined by

$$n = N^{-1} \sum_j m_j, \tag{47}$$

which means

$$1 - 2n = N^{-1} \sum_j (-1)^{n_j}, \tag{48}$$

we have from Eq. (46)

$$\zeta = |1 - 2n|, \tag{49}$$

$$\psi_l = \begin{cases} 2l\pi/k & \text{for } n < 1/2, \\ (2l+1)\pi/k & \text{for } n > 1/2, \end{cases} \tag{50}$$

where $l \in \mathbb{Z}$. Then the choice of the set $\{m_j\}$ is not sufficient to specify the set $\{\varphi_j\}$, because the constant ψ can assume some different values. This fact is connected with the symmetry structure of the potential energy surface: the different values of ψ_l correspond to the symmetry-related critical points under the group C_{kv}.

We can then state that all the critical points with $\zeta \neq 0$-whose energy $v \neq \Delta$—have the form

$$\tilde{\varphi}_j^{\mathbf{m},l} = [m_j \pi - (k-1)\psi_l]_{\mathrm{mod}\ 2\pi}. \tag{51}$$

The Hessian matrix is given by

$$\mathcal{H}_{ij}^k = \Delta k\ \mathrm{Re}[N^{-1}(k-1)(c+is)^{k-2} e^{i(\varphi_i+\varphi_j)} + \delta_{ij}(c+is)^{k-1} e^{(i\varphi_i)}]. \tag{52}$$

In the thermodynamic limit it becomes diagonal

$$\mathcal{H}_{ij}^k = \delta_{ij} \Delta k \zeta^{k-1} \cos[\psi(k-1) + \varphi_i]. \tag{53}$$

One cannot *a priori* neglect the contribution of the off-diagonal terms to the eigenvalues of $\mathcal{H}$, but we have numerically checked that their contribution change at most the sign of only one eigenvalue over N: we note that in the case of the mean-field XY model this result has been proven explicitly [7]. Neglecting the off-diagonal contributions, the eigenvalues of the Hessian calculated in the critical point $\tilde{\varphi}$ are obtained substituting Eq. (51) in Eq. (53):

$$\lambda_j = (-1)^{m_j} \Delta k \zeta^{k-1}, \tag{54}$$

so the index of the critical point is simply the number of $m_j = 1$ in the set $\mathbf{m}$; we can identify the quantity $n(\tilde{\varphi})$ given by Eq. (47) with the *fractional index* ν/N of the critical point $\tilde{\varphi}$. Then, from Eqs. (4), (49), and (50) we get a relation between the fractional index $n(\tilde{\varphi})$ and the potential energy $v(\tilde{\varphi}) = V(\tilde{\varphi})/N$ at each critical point $\tilde{\varphi}$:

$$n(v) = \frac{1}{2}\left[1 - \mathrm{sgn}\left(1 - \frac{v}{\Delta}\right)\left|1 - \frac{v}{\Delta}\right|^{1/k}\right]. \tag{55}$$

Moreover, the number of critical points of given index ν is simply the number of way in which one can choose ν times 1 among the $\{m_j\}$, see Eq. (51) , multiplied for a constant $\mathcal{A}_k$ that takes into account the degeneracy introduced by Eq. (50).

We have then completely characterized the critical points with $\zeta \neq 0$. Now we are going to argue that, in order to compute the Euler characteristic of the manifolds M_v, we can neglect the critical points with $\zeta = 0$, thus showing that the knowledge of the critical points considered so far is sufficient. The critical points with $\zeta = 0$ are degenerate: the Hessian vanishes at these points. This means that the potential energy is no longer a proper Morse function when $v \geqslant \Delta$, and we could use its critical points to compute the Euler characteristic of the manifolds M_v only when $v < \Delta$. To overcome this difficulty we reason as follows. Morse functions are dense in an open set of the space of smooth functions: this means, in practice, that if a function f is *not* a Morse function, any small perturbation will make it a proper Morse function [19], and we can consider, as our Morse function, the function $\tilde{V}_k$, i.e., the potential energy plus a linear term which can made as small as we want

$$\tilde{V}_k = V_k + \sum_{i=1}^{N} h_i \varphi_i, \tag{56}$$

where $h \in \mathbb{R}^N$. The perturbation changes only slightly the critical points with $\zeta \neq 0$, but completely removes the points with $\zeta = 0$ for any $h \neq 0$, no matter how small. All the critical points of this function are given by the solutions of the equations

$$\sin[(k-1)\psi + \varphi_j] = h_j \quad \forall\, j = 1, \ldots, N, \tag{57}$$

which are only a slight deformation of Eqs. (44), so that provided all the h's are very small the numerical values of critical points and critical levels will essentially coincide with those computed so far, in the case $h = 0$ but assuming $\zeta \neq 0$.

The fractional index $n = \nu/N$ of the critical points is a well defined monotonic function of their potential energy v, given by Eq. (55), and the number of critical points of a given

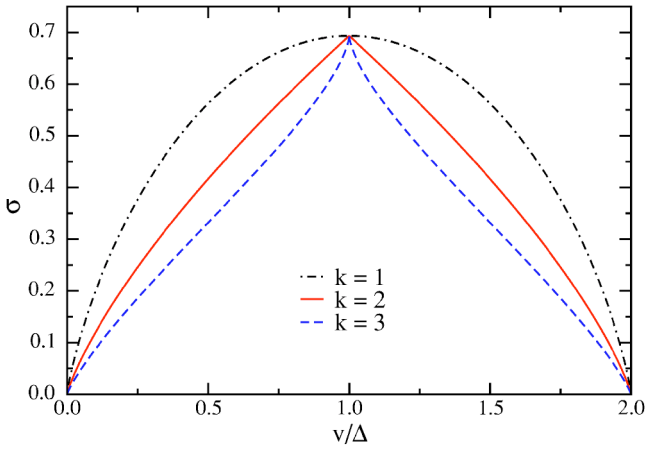

FIG. 7. Logarithmic Euler characteristic of the M_v manifolds $\sigma(v)$ (see text) as a function of the potential energy v. The phase transition is signaled as a singularity of the first derivative at $v_c=\Delta$; the sign of the second derivative around the singular point allows to discriminate between transitions of different order. The region $v>\Delta$, in which $\sigma'(v)<0$, in not reached by the system (see text).

index ν is $\mathcal{A}_k\binom{N}{\nu}$. Then the Morse indexes $\mu_\nu(M_v)$ of the manifold M_v are given by $\mathcal{A}_k\binom{N}{\nu}$ if $\nu/N \leqslant n(v)$ and 0 otherwise, and the Euler characteristic is

$$\chi(v) = \mathcal{A}_k \sum_{\nu=0}^{Nn(v)} (-1)^\nu \binom{N}{\nu} = \mathcal{A}_k (-1)^{Nn(v)} \begin{bmatrix} N-1 \\ Nn(v) \end{bmatrix}, \tag{58}$$

using the relation $\Sigma_{\nu=0}^{m}(-1)^{N}\binom{N}{\nu}=(-1)^{m}\binom{N-1}{m}$.

In Fig. 7 we plot $\sigma(v)=\lim_{N\to\infty}(1/N)\log|\chi(v)|$, that, from Eq. (58) , is given by

$$\sigma(v) = -n(v)\log n(v) - [1-n(v)]\log[1-n(v)]. \tag{59}$$

It has to be stressed that $\sigma(v)$ is a purely *topological* quantity, being related only to the properties of the potential energy surface defined by $V_k(\varphi)$, and, in particular, to the energy distribution of its saddle points. From Fig. 7 we can see that there is an evident signature of the phase transition in the analytic properties of $\sigma(v)$. First, we observe that the region $v>\Delta$ is never reached by the system, as discussed before and showed in Figs. 5 and 6 as to the microcanonical case, and in Figs. 2 and 3 as to the canonical case; this region is characterized by $\sigma'(v)<0$. The main observations are that: (i) for $k=1$, where there is no phase transition, the function $\sigma(v)$ is analytic; (ii) for $k=2$, when we observe a second order phase transition, the first derivative of $\sigma(v)$ is discontinuous at $v_c=v(e_c)=\Delta$, and its second derivative is *negative* around the singular point; (iii) for $k\geqslant 3$ the first derivative of $\sigma(v)$ is also discontinuous at the transition point $v_c=\Delta$, but its second derivative is *positive* around v_c. In this case *a first order transition takes place*. Therefore the investigation of the potential energy topology, via $\sigma(v)$, allows us to establish not only the location but also the order of the phase transitions, without introducing any statistical measure.

The previous results suggest us to conjecture that there is a relation between the thermodynamic entropy of the system and the topological properties of the potential energy landscape, as probed by $\sigma(v)$. We recall that the presence of a first order transition with a discontinuity in the energy is generally related [20] to a region of negative specific heat, i.e., of positive second derivative of the entropy. Thus, it seems that at least around the transition point the thermodynamic entropy and $\sigma[v(e)]$ are closely related: more precisely, it seems that the jump in the second derivative of $s(e)$ is determined by the jump in the second derivative of $\sigma[v(e)]$. Then it should be possible to write

$$s(e) \sim \sigma(v(e)) + \mathcal{R}(e) \tag{60}$$

where $\mathcal{R}(e)$ is analytic (or, at least, C^2) around the transition point.

In Sec. III we explain how such a link between thermodynamics and topology could be obtained. But before doing so we show a different way of looking at the topology of the submanifolds of configuration space defined by the potential energy.

D. Topology of the order parameter space

A feature of many mean-field models (although not of all of them) is that the potential energy can be written as a function of a collective variable, whose statistical average is the order parameter. In the case of the k-trigonometric model this variable is the two-dimensional "magnetization" vector defined as $\mathbf{m}=(c,s)$, where [see Eqs. (5)]:

$$c = \frac{1}{N}\sum_{i=1}^{N} \cos(\varphi_i),$$

$$s = \frac{1}{N}\sum_{i=1}^{N} \sin(\varphi_i). \tag{61}$$

Written in terms of (c,s), the potential energy is a function defined on the unitary disk in the real plane, which is given by [see Eq. (4)]:

$$V_k(c,s) = N\Delta\left\{1 - \sum_{n=0}^{[k/2]} \binom{k}{2n} (-1)^n c^{k-2n} s^{2n}\right\}. \tag{62}$$

In the particular cases $k=1,2,3$ the potential energy V_k reads as

$$V_1(c,s) = N\Delta(1-c), \tag{63}$$

$$V_2(c,s) = N\Delta(1-c^2+s^2), \tag{64}$$

$$V_3(c,s) = N\Delta(1-c^3+3cs^2), \tag{65}$$

and it is then natural to investigate the topology of the M_v's seen as submanifolds of the unitary disk in the plane, i.e., we now consider the submanifolds

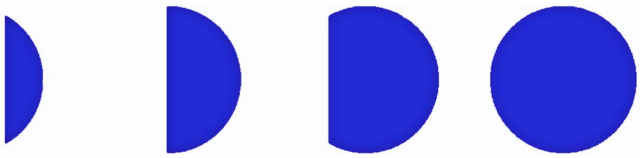

FIG. 8. The submanifolds $\mathcal{M}_v$ in the case $k=1$ for $v=0.5\Delta,\Delta,1.5\Delta,2\Delta$ (from left to right). All the submanifolds are topologically equivalent to a single disk.

$$\mathcal{M}_v \equiv \{(c,s) \in D^2 | V_k(c,s) \leqslant Nv\}, \tag{66}$$

where $D^2 \equiv \{(c,s) \in \mathbb{R}^2 | c^2+s^2 \leqslant 1\}$. The $\mathcal{M}_v$'s are nothing but the M_v's projected onto the magnetization plane.

The topology of these manifolds can be studied directly, by simply drawing them. In the case $k=1$, where no phase transition is present, no topology changes occur in the $\mathcal{M}_v$'s, i.e., all of them are topologically equivalent to a single disk D^2 (Fig. 8). When $k=2,3$, and a phase transition is present, there is a topology change precisely at $v_c=\Delta$, where k disks merge into a single disk (see Figs. 9 and 10). The detail of the transition, i.e., the number of disks which merge into one, clearly reflects the nature of the symmetry breaking for the particular value of k considered (similar pictures are obtained for $k>3$). Thus, when projected onto the order parameter space, the correspondence between topology changes and phase transitions becomes one-to-one (this was already found in Ref. [21] for the mean-field XY model); however, at variance with the study of the topology of the "full" M_v's, no direct way to discriminate between first and second-order transitions seems available in this picture.

III. TOPOLOGY AND THERMODYNAMICS: A DIRECT LINK

We now show how it is possible to establish a general relationship between topology and thermodynamics. This can be achieved by improving some preliminary results on the subject reported in Refs. [22,23].

Consider a generic classical system described by a Hamiltonian

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

where $q=(q_1,\ldots,q_N)$ and the symbols have standard meaning. Then consider the microcanonical entropy $S(E)$ defined as

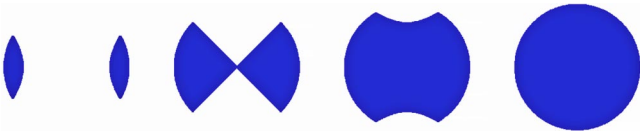

FIG. 9. The submanifolds $\mathcal{M}_v$ in the case $k=2$ for $v=0.5\Delta,\Delta,1.5\Delta,2\Delta$ (from left to right). As $v<v_c=\Delta$ the submanifolds are topologically equivalent to two disconnected disks, while as $v>v_c$ they are equivalent to a single disk.

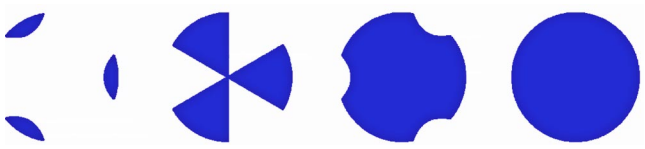

FIG. 10. The submanifolds $\mathcal{M}_v$ in the case $k=3$ for $v=0.5\Delta,\Delta,1.5\Delta,2\Delta$ (from left to right). As $v<v_c=\Delta$ the submanifolds are topologically equivalent to three disconnected disks, while as $v>v_c$ they are equivalent to a single disk.

$$S(E) = \frac{k_B}{N}\log\,\Omega_\nu(E), \tag{67}$$

where $\nu=2N-1$, where we shall put $k_B=1$ and where

$$\Omega_\nu(E) = \frac{1}{N!}\int_{\Sigma_E}\frac{d\sigma}{\|\nabla H\|}, \tag{68}$$

with $\|\nabla H\|=\{\Sigma_i p_i^2+[\nabla_i V(q)]^2\}^{1/2}$, i.e., Ω_ν is the microcanonical density of states. Here Σ_E is the constant-energy hypersurface in the $2N$-dimensional phase space Γ corresponding to the total energy E, that is $\Sigma_E=\{(p_1,\ldots,p_N,q_1,\ldots,q_N) \in \Gamma | H(p,q)=E\}$.

From the general derivation formula [24]:

$$\frac{d^k}{dE^k}\int_{\Sigma_E}\alpha\, d\sigma = \int_{\Sigma_E} A^k(\alpha) d\sigma, \tag{69}$$

where α is an integrable function and A is the operator

$$A(\alpha) = \frac{\nabla}{\|\nabla H\|}\left(\alpha\frac{\nabla H}{\|\nabla H\|}\right)$$

the following result is worked out:

$$\frac{d\Omega_\nu(E)}{dE} = \frac{1}{N!}\int_{\Sigma_E}\frac{d\sigma}{\|\nabla H\|}\frac{M_1^\star}{\|\nabla H\|} + \mathcal{O}\left(\frac{1}{N}\right), \tag{70}$$

where $M_1^\star=\nabla(\nabla H/\|\nabla H\|)$. $M_1^\star$ is directly proportional to the mean curvature M_1 of Σ_E seen as a submanifold of $\mathbb{R}^N$ [25] according to the simple relation $M_1=-M_1^\star/(2N-1)$. By integrating equation Eq. (70) we obtain the following equivalent expression for $\Omega_\nu(E)$:

$$\Omega_\nu(E) = \frac{1}{N!}\int_0^E d\eta\int_{\Sigma_\eta}\frac{d\sigma}{\|\nabla H\|}\frac{M_1^\star}{\|\nabla H\|} = \frac{1}{N!}\int_{M_E} d\mu\frac{M_1^\star}{\|\nabla H\|} \tag{71}$$

and then, at large N, considering that the volume measure $d\mu$ concentrates on the boundary Σ_E, we write

$$\frac{1}{N!}\int_{M_E} d\mu\frac{M_1^\star}{\|\nabla H\|} \simeq \frac{(\delta E)}{N!}\int_{\Sigma_E}\frac{d\sigma}{\|\nabla H\|}\frac{M_1^\star}{\|\nabla H\|} \simeq \frac{(\delta E)}{N!}\langle\|\nabla H\|^{-1}\rangle\int_{\Sigma_E}\frac{d\sigma}{\|\nabla H\|}M_1^\star, \tag{72}$$

where, in the last approximate replacement, we have used that $\|\nabla H\|$ is positive and only very weakly varying at large N.

By means of Hölder's inequality for integrals we get

$$\int_{\Sigma_E} \frac{d\sigma}{\|\nabla H\|} M_1^\star \leqslant \left(\int_{\Sigma_E} \frac{d\sigma}{\|\nabla H\|} |M_1^\star|^N \right)^{1/N} \left(\int_{\Sigma_E} \frac{d\sigma}{\|\nabla H\|} \right)^{(N-1)/N},$$

the sign of equality being better approached when $M_1^\star$ is everywhere positive. Hence, using Eqs. (68), (71), and (72)

$$\Omega_\nu(E) \leqslant [\Omega_\nu(E)]^{(N-1)/N} \left(\frac{1}{N!} \int_{\Sigma_E} \frac{d\sigma}{\|\nabla H\|} |M_1^\star|^N \right)^{1/N} \frac{\delta E}{\langle \|\nabla H\| \rangle} \tag{73}$$

and assuming that a regular deformation factor $d(E)$ exists [29] such that we can write

$$[\Omega_\nu(E)]^{1/N} = \frac{d(E)\delta E}{\langle \|\nabla H\| \rangle} \left(\frac{1}{N!} \int_{\Sigma_E} \frac{d\sigma}{\|\nabla H\|} |M_1^\star|^N \right)^{1/N} \tag{74}$$

we then obtain

$$\Omega_\nu(E) = \frac{2^N [d(E)]^N (\delta E)^N}{\langle \|\nabla H\| \rangle^{N+1}} \int_{\Sigma_E} d\sigma \left[|K_G| + \frac{\mathcal{R}(E)}{2^N N!} \right], \tag{75}$$

where we have used $2^{-N}|M_1^\star|^N = (\kappa_1 + \kappa_2 + \cdots + \kappa_N)^N = N!|K_G| + \mathcal{R}(E)$, with $\kappa_1, \ldots, \kappa_N$ the principal curvatures of Σ_E, and K_G is the Gauss-Kronecker curvature of Σ_E, $K_G = \Pi_{i=1}^N \kappa_i$. $\mathcal{R}(E)$ is a remainder. Again we have used that $\|\nabla H\|$ is only very weakly varying at large N and that it is always positive.

According to the Chern-Lashof theorem [26]

$$\int_{\Sigma_E} d\sigma |K_G| = \mathrm{vol}(\mathbb{S}_1^{N-1}) \sum_{i=0}^{N} \mu_i(\Sigma_E) \tag{76}$$

where $\mathbb{S}_1^{N-1}$ is an $(N-1)$-dimensional hypersphere of unit radius and $\mu_i(\Sigma_E)$ are the Morse indexes of Σ_E which are defined exactly as those of the M_v's seen in the previous sections, i.e., as the number μ of critical points of index i on a given level set $\Sigma_E = H^{-1}(E)$; a critical point is a point where $\nabla H = 0$, the index i of a critical point is the number of negative eigenvalues of the Hessian of H computed at the critical point.

Finally the entropy per degree of freedom reads as

$$S(E) = \frac{1}{N} \log \Omega_\nu(E) = \frac{1}{N} \log \left[\mathrm{vol}(\mathbb{S}_1^{N-1}) \sum_{i=0}^{N} \mu_i(\Sigma_E) + \int_{\Sigma_E} d\sigma \frac{\mathcal{R}(E)}{2^N N!} \right] + \frac{1}{N} \log \frac{2^N [d(E)]^N (\delta E)^N}{\langle \|\nabla H\| \rangle^{N+1}}. \tag{77}$$

The meaning of Eq. (77) is better understood if we consider that the Morse indexes $\mu_i(M)$ of a differentiable manifold M are related to the Betti numbers $b_i(M)$ of the same manifold by the inequalities

$$\mu_i(M) \geqslant b_i(M). \tag{78}$$

The Betti numbers are fundamental *topological invariants* [18] of differentiable manifolds; they are the diffeomorphism-invariant dimensions of suitable vector spaces (the de Rham's cohomology spaces), thus they are integer numbers. The equality sign holds only for the so-called perfect Morse functions, which are rare, however, at large dimension we can safely replace Eq. (78) with $\mu_i(M) \simeq b_i(M)$ (see, e.g., Ref. [7]).

Equation (77), rewritten as

$$S(E) \simeq \frac{1}{N} \log \left[\mathrm{vol}(\mathbb{S}_1^{N-1}) \sum_{i=0}^{N} b_i(\Sigma_E) + \int_{\Sigma_E} d\sigma \frac{\mathcal{R}(E)}{2^N N!} \right] + \frac{1}{N} \log \frac{2^N [d(E)]^N (\delta E)^N}{\langle \|\nabla H\| \rangle^{N+1}}, \tag{79}$$

links topological properties of the *microscopic* phase space with the *macroscopic* thermodynamic potential $S(E)$.

In particular, even though the function $\mathcal{R}(E)$ is unknown, sudden changes of the topology of the hypersurfaces Σ_E [reflected by the energy variation of $\Sigma b_i(\Sigma_E)$] necessarily affect the energy variation of the entropy.

Finally, we resort to the fact that—at large N—the volume measure of Σ_E concentrates on $\mathbb{S}^{N-1}_{\langle 2K \rangle^{1/2}} \times M_{\langle V \rangle}$, where $\mathbb{S}^{N-1}_{\langle 2K \rangle^{1/2}} = \{(p_1, \ldots, p_N) | \Sigma p_i^2 = \langle 2K \rangle\}$ is the kinetic energy hypersphere and $M_{\langle V \rangle} = \{(q_1, \ldots, q_N) | V(q) \leqslant \langle V \rangle\}$, so that Σ_E can be approximated by this product manifold, and we resort to the Kunneth formula [18] for the Betti numbers of a product manifold $A \times B$, i.e.,

$$b_i(A \times B) = \sum_{j+k=i} b_j(A) b_k(B) \tag{80}$$

which, 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 $i = 1, \ldots, N-1$, and $b_j(\Sigma_E) = b_j(M_v)$ for $j = 0, N$, since all the Betti numbers of an hypersphere vanish but b_0 and b_N which are equal to 1 [18]. Eventually we obtain

$$S(v) \simeq \frac{1}{N} \log \left\{ \mathrm{vol}(\mathbb{S}_1^{N-1}) \left[b_0 + \sum_{i=1}^{N-1} 2b_i(M_v) + b_N \right] + \tilde{\mathcal{R}}[E(v)] \right\} + \frac{1}{N} \log \frac{2^N [d(E)]^N (\delta E)^N}{\langle \|\nabla H\| \rangle^{N+1}}, \tag{81}$$

where $\tilde{\mathcal{R}}[E(v)]$ stands for the integral on the product manifold of the remainder which appears in Eq. (79). The equation earlier makes explicit the fact that the kinetic energy term of a standard Hamiltonian is topologically trivial.

From this equation we see that a fundamental topological quantity, the sum of the Betti numbers of the submanifolds $M_v = \{(q_1, \ldots, q_N) \in \mathbb{R}^N | V(q) \leqslant v\}$ of configuration space, is related, although with some approximation, to the thermodynamic entropy of the system.

While a relationship between topology and thermodynamics exists, as is shown by both Eqs. (81) and (77), an analytic formula linking the Euler characteristic to thermodynamics has not been found yet and is unlikely to exist. Therefore, in those cases allowing the analytic computation of the Morse indexes (as for the models tackled in this paper), besides the computation of the Euler characteristic through the formula (39), we can use the Morse indexes to replace the sum $[b_0$

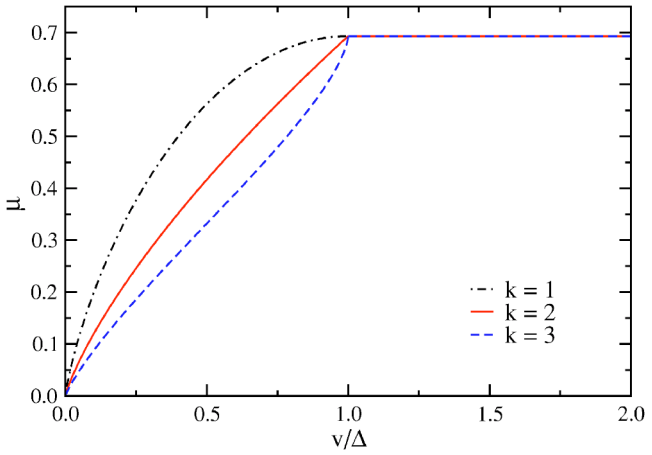

FIG. 11. Logarithm of the sum of the Morse indexes divided by N, $\mu=(1/N)\log\left[\mu_0+2\Sigma_{i=1}^{N-1}\mu_i(M_v)+\mu_N\right]$ of the manifolds M_v vs the energy density v, scaled with Δ, for $k=1,2,3$.

$+\Sigma_{i=1}^{N-1}2b_i(M_v)+b_N]$ in Eq. (81) with $[\mu_0+\Sigma_{i=1}^{N-1}2\mu_i(M_v)+\mu_N]$, having resorted again to the estimate $b_i(M)\simeq\mu_i(M)$. Then we can plot this sum, that we shall denote by μ, against the potential energy density for the three different cases considered: $k=1,2,3$. The result is shown in Fig. 11, where sharp differences are evident between the three situations: (i) $k=1$, absence of any phase transition, in which case the pattern of μ vs v is smooth; (ii) $k=2$, second-order phase transition, in which case the pattern of μ vs v displays a sharp nondifferentiable change at the phase transition point; (iii) $k=3$, first-order phase transition, in which case the pattern of μ vs v again displays a sharp nondifferentiable change at the phase transition point which is approached from the left with an opposite concavity with respect to the second-order transition case. Likewise the Euler characteristic, the quantity μ is in one-to-one correspondence with topology changes of the manifolds M_v, but μ has the advantage of being directly related with thermodynamic entropy.

Both the general analytic result of Eq. (81) and the particular analytic result obtained for the kTM and reported in Fig. 11 are of great relevance in view of a deeper understanding of the relationship between topology changes of configuration space and phase transitions: further work is ongoing along this direction.

As a final comment, let us remark that the clearcut differences among the three different cases in Fig. 11 are detected *prior to* and *independently of* the definition of any statistical measure in configuration space: the relevant information about the macroscopic physical behavior is already contained in the microscopic interaction potential itself and concealed in its way of shaping configuration space submanifolds.

IV. CONCLUDING REMARKS

We have presented a mean-field model whose thermodynamics is exactly solvable in both the canonical and the microcanonical ensemble: the model depends on a parameter k and exhibits no transitions, a continuous phase transition and a discountinuous one, in the cases $k=1$, $k=2$, and $k\geqslant 3$, respectively. For this model, a clear and sharp relation between the presence of a phase transition and a particular topology change in the submanifolds of the N-dimensional configuration space is analytically worked out: this correspondence becomes one-to-one if we look at the submanifolds of a reduced two-dimensional configuration space spanned by collective variables. Moreover, not only the presence and the location in energy of the transition can be inferred by looking at the behavior of topological quantities: also the order of the transition is related to the behavior of a topological invariant of the earlier mentioned submanifolds, their Euler characteristic. This suggests that topological quantities are linked in general to thermodynamic observables. Such a general link, although based on some approximations, has been derived in the final section of the paper.

The results presented here confirm the validity and the potential of the topological approach to phase transitions, which has recently received a rigorous background via the proof of a theorem [8] stating that, for systems with short-ranged interactions, topology changes in the submanifolds of configuration space are a *necessary* condition for a phase transition to take place. The model we studied here is not short ranged, thus the theorem might probably be extended to a more general class of systems. However, we would like to mention the case of a mean-field model, the fully coupled φ^4 model, which has been recently studied [27], and where the relation between the topology changes in the submanifolds of the configuration space and the phase transition is less straightforward. Further work is then needed to assess the full potential and the limits of the topological approach to phase transitions.

Concerning in particular first-order phase transitions, it would be very interesting to test the topological approach of the present paper in models with more realistic interactions, i.e., described by potentials with a hard-core repulsion, short ranged, and in two or three space dimensions. In other words, it would be interesting to find the topological counterpart of the phenomena of freezing and condensation. On general grounds, and in particular on the basis of the theorem in Ref. [8], topology—in the sense of the present paper—is expected to play a role also in these systems. Consider, e.g., inverse power potentials: as in this case the theorem in Ref. [8] applies, the submanifolds M_v's and Σ_v's must undergo a nontrivial and energy-depending topology change at the first-order transition point. However, how this topology change is shaped remains unknown and deserves investigation. On the other hand, finding all the critical points of a short-ranged potential energy function, in two or three dimensions, seems at present a very hard task, from both analytical and numerical points of view. The situation is not better in the case of hard spheres systems, that is of entropy driven phase transitions. In this case, the (singular) interaction potential cannot play any longer the role of Morse function, what does not mean that the connection between topology and phase transitions is lost, but that in this case other Morse functions are to be used to probe and characterize topology (a possible choice could be the sum of all the pairwise euclidean distances between the hard spheres of a system: it is real valued, it has a minimum when the density is maximum, that is for close packing; the discussion of nondegeneracy is more in-

volved and here would be out of place). The spatial density of spheres should replace energy in the role of control parameter. This is still a completely open field of investigation.

In conclusion, applying the topological approach to "real" first-order transitions will probably need a substantial advance in both the analytical and numerical methodologies.

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[28] Mean-field models with long-range interactions, like those to be analyzed in the present paper, do not rigorously fulfill the hypotheses of the theorem proved in Ref. [8]; the fact that we do find a correspondence between the phase transition and a particular topology change also for these models, as already found in other models with long-range interactions, suggests that the theorem could be probably extended to a wider class of systems, which, however, would not necessarily include all the possible kinds of models with long-range, mean-fieldlike interactions (see also the discussion in Sec. IV).
[29] This assumption is reasonable in the light of the results reported in Ref. [22].