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Topology and Phase Transitions: The Case of the Short Range Spherical Model

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We characterize the topology of the phase space of the Berlin-Kac spherical model in the context of the so called Topological Hypothesis, for spins lying in hypercubic lattices of dimension d. For zero external field we are able to characterize the topology exactly, up to homology. We find that, even though there is a continuum of changes in the topology of the corresponding manifolds, for $d \geq 3$ there are abrupt discontinuities in some topological functions that could be good candidates to associate with the phase transitions that occur at the thermodynamic level. We show however that these changes *do not* coincide with the phase transitions and conversely, that no topological discontinuity can be associated to the points where the phase transitions take place. At variance with what happens in the Mean Field version of this same model, we show that these abrupt topological changes *are* accessible thermodynamically. We conclude that, even in short range systems, the topological mechanism does not seem to be responsible for the triggering of a phase transition. We also analyze the case of spins connected to a macroscopic number of (but not all) neighbors, and find that, similar to the results found for the fully connected version, in this case the topological hypothesis seems to hold: the phase transition coincides with an accumulation point of the topological changes present in configuration space. The question of the ensemble equivalence in the short range spherical model is also considered.

KEY WORDS: topology, statistical mechanics, spherical model, toplogical hypothesis, ensemble equivalence

1. INTRODUCTION

Phase transitions (PTs) remain one of the most intriguing and interesting phenomena in physics. One of the aims of statistical mechanics has been to be able to

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characterize and predict the conditions for the occurrence of PTs for very distinct theoretical models. Mathematically, a phase transition is signaled by the loss of analyticity of some thermodynamic function.[1,2] Because it is based on the analysis of thermodynamic functions, this characterization of PT's is a macroscopic one. From a more fundamental point of view one would like to investigate whether a microscopic characterization exists, that can emerge directly from the microscopic interactions, i.e., *prior* to any definition of *statistical* measure. If such a characterization were possible, it could eventually enable one to classify the microscopic interactions among those leading to continuous or discontinuous phase transitions, or no phase transitions at all.

Recently, a new characterization of PTs has been put forward,[3] that aims at detecting the PTs directly at the level of the phase space topology of the system. Notice that in this case one is studying the problem at a more fundamental level, and it is not necessary to resort to thermodynamics or statistical ensembles. In this new method one studies the topology of the configuration space Γ of the system, defined by the potential energy function $V(\mathbf{x})$ and determining the changes that take place in the potential energy submanifolds (PES) $M_v = \{\mathbf{x} \in \Gamma : V(\mathbf{x})/N < v\}$ as the parameter v is increased. A topological transition (TT) is said to take place at c if the manifolds $M_{c-\epsilon}$ and $M_{c+\epsilon}$ are not homeomorphic. The idea is that somehow TTs must be related to PTs. In Ref. 4 it is stated that "at their deepest level PTs of a system are due to a change of the topology of the configuration space." This is known as the *Topological Hypothesis*. Notice that even if a TT at a certain v can be unambiguously related to a PT, one still needs to resort to thermodynamics to determine at which temperature this v is reached.

The relationship between PTs and TTs has been studied for several models in the last years. It has been shown that interesting differences arise in this relation between systems with long range interactions (i.e. in the Mean Field (MF) limit) and the Short Range (SR) versions of them. For example, in the XY model[4] TTs are found both in the MF and the SR version in dimension $d = 1$, whereas a PT is present only in the MF case. This fact made clear that probably only some class of topology changes could be responsible for the triggering of a phase transition, it was necessary to better characterize the TT's in order to understand under what conditions these can induce or be correlated with PTs. Using the changes in the Euler characteristic as a quantitative measure of a TT, it was found that a *macroscopic* change happens in the MF model at exactly the same point (potential energy level) where statistical mechanics predicts a phase transition, while such an abrupt topology change is absent in the one-dimensional model. In a similar mean field model, called *k-trigonometric*,[5] the topological hypothesis seems to work even in the case of first order transitions. Nevertheless, ensemble equivalence is not fulfilled for this case, as expected, and, moreover, the definition of the transition point in energy becomes ambiguous for first order PTs. Hence, the connection with the topology changes is not straightforward.[6]

For the lattice ϕ^4 model, numerical work has shown a correlation between TTs and PTs in the SR version in dimension $d = 2$.[7] In the mean field version both TTs and PTs exist but they do not coincide[8,9] (in Ref. 8 however, it is suggested that TTs could be related to the properties of the inherent saddles of the potential energy landscape).

In these works the characterization of the phase space is done using the index (i.e. the number of negative eigenvalues of the Hessian) of the critical points of the potential energy function. These can be *indirectly* related to the topology through Morse theory.[10] In the frame of this theory the only topological invariant that can be directly calculated is the Euler characteristic, which is not enough to determine the topology of the space (not up to homology, at least). The characterization through the Euler characteristic limits the topological approach. One of the questions that remains is, for example, whether PTs can be related to a change in a *different* invariant.

A somewhat different approach was followed in two recent works on non-confining, short ranged, potentials. For these functions, one of the possible topological transitions is the loss of compactness of the manifold at a certain v. For a model of DNA denaturation it was shown that this loss of compactness induces a PT.[11] On the other hand, for one of the variants of the Burkhardt model[12] the breaking of compactness was shown to be *insufficient* to induce a PT.

In an important contribution,[13] Franzosi, Pettini and Spinelli have proved that for smooth, confining, stable and short ranged potentials, a TT is a *necessary* condition for the appearance of a PT. This general and important result loses part of its relevance for short ranged systems for which in the limit of infinite size there is a continuum of TTs, as is the case of the potentials mentioned.

In the mean field version of the spherical model,[14] a correlation was found between the TT and the PT. Interestingly, in the case of nonvanishing external field there is no PT, but the phase space displays a TT at energies that cannot be thermodynamically reached. More recently, Kastner[6] showed that this behavior could be understood by noting that the model has partial equivalence of ensembles: whereas in the canonical ensemble there is a continuous phase transition, in the more fundamental microcanonical ensemble there is no phase transition within the allowed support of the entropy function.

In a recent letter[15] we addressed the case of the short range spherical model.[16] We showed that the phase transitions occurring for $d \geq 3$ cannot be related to any *particularly strong* change in the homology of the potential energy manifolds at v_c. On the other hand, we showed that the phase space has some rather abrupt changes in topology that are not related to PTs.

Here we present a detailed derivation of the results advanced in Ref. 15. Using tools from topology theory and taking profit of the relative simplicity of the phase space of the spherical model, we are able, in the case of vanishing field, to determine its topology *exactly* (up to homology). For nonvanishing field we cannot characterize the topology completely for all v, but we are at least able to show that a very abrupt change in the topology happens that does not have a corresponding PT. At variance with what happens for the MF version these topological changes, although unrelated to the PTs, *are thermodynamically accessible*.

In Sec. 2 the d-dimensional nearest neighbors spherical model is introduced. In Sec. 3 we review the relevant facts of the thermodynamics of the model, that was studied in depth by Berlin and Kac in their seminal work.[16] The model displays a phase transition only in the case of $d \geq 3$ and vanishing field. In Sec. 4 we study the topology of phase space, showing that the manifolds M_v are homotopically equivalent to spheres whose dimension can be related to the index of the critical solutions. We show that some derivatives of the index, as a function of v, display several discontinuities. We argue that these points of discontinuity are the likely candidates to be identified with PTs, in case these latter were present. However, it is shown that none of them correspond to the PTs observed for $d \geq 3$. Furthermore, it is also shown that when an external field is turned on, there appear abrupt discontinuities in *the index itself*. But no PT is associated to this abrupt topological changes. In Sec. 5 we prove the equivalence between the microcanonical and canonical ensembles for the short range spherical model and, therefore, the same conclusions regarding the lack of correlation between the topological mechanism and the PTs apply to the microcanonical ensemble. In Sec. 6 we briefly comment on the case of long range connections that do not span the whole system. In the last section some conclusions and perspectives for future reasearch are drawn.

2. THE MODEL

The spherical model is defined by N spins placed in a d-dimensional lattice, whose potential energy in an external field H is given by:

$$V = -\frac{1}{2} \sum_{ij} J_{ij}\, \epsilon_i \epsilon_j - H \sum_i \epsilon_i, \tag{1}$$

where the interaction matrix element J_{ij} gives the strength of the interaction between spins i and j. The spin variables are real and are constrained to lie on the sphere $\Gamma = \mathbb{S}^{N-1} = \{\epsilon \in \mathbb{R}^N : \sum_i \epsilon_i^2 = N\}$. This is equivalent to considering that the potential is infinite outside this sphere.

Since the work of Berlin and Kac[16] in which they study hypercubic lattices of spins connected to their first neighbours, the thermodynamics of this system has been studied also for other choices of the interaction matrix.[17,18] In Sec. 6 we briefly comment the case of lattices with macroscopic but not full connectivities (the topology of the fully connected model has already been studied in Ref. 14).

3. THERMODYNAMICS

For a detailed discussion of the thermodynamics of the spherical model the reader is refered to the original work of Berlin and Kac.[16] Here we only quote the main points relevant to our analysis of the topology of this model. In a hypercubic lattice in d dimensions each spin interacts only with its $2d$ closest neighbours. The strength of the pairwise interaction is given by J. The thermodynamic functions can be obtained from the (configurational) partition function, defined as:

$$Q_N(\beta, H) = A_N^{-1} \int_{\mathbb{S}^{N-1}} d\epsilon_1, \ldots, d\epsilon_N \exp\left(-\beta V(\epsilon_1, \ldots, \epsilon_N)\right), \tag{2}$$

where A_N is just the surface of the $(N-1)$-dimensional sphere (with radius $\sqrt{N}$) and accounts for the proper normalization of the partition function.

After some algebra[16] one arrives at an integral over a parameter z which, in the limit of large N can be evaluated using the saddle point method. The saddle point equation is:

$$4K = \frac{df_d(z)}{dz} + K(H/J)^2/(z - \lambda_1/2) \tag{3}$$

where $K = \beta J/2$, λ_1 is the largest eigenvalue of the adjacency matrix of the lattice, and $f_d(z)$ is defined by

$$\begin{aligned} f_d(z) &= \lim_{N\to\infty} N^{-1} \sum_{j=2}^{N} \ln(z - \lambda_j/2) \\ &= (2\pi)^{-d} \int_0^{2\pi} d\omega_1, \ldots, d\omega_d \ln\left(z - \sum_{i=1}^{d} \cos\omega_i\right) \end{aligned} \tag{4}$$

where d is the dimension of the lattice, and $2\sum_{i=1}^{d} \cos\omega_i = \lambda(\omega)$ are the eigenvalues of the adjacency matrix in the infinite N limit. The critical temperature, when it exists, is the one obtained from Eq. (3) for the saddle point solution $z_c = \lambda_1/2$. It is easy to show that for a nonvanishing field, this solution implies $K \to \infty$, i.e. $T_c = 0$, meaning that in this case no phase transition is possible at any d. For temperatures larger than the critical, there is always a solution $z > \lambda_1/2$. For vanishing external field there can be a finite critical temperature. For $T < T_c$, it can be shown that the saddle point 'sticks,' i.e., $z = \lambda_1/2$ for all values of T smaller than the critical. For $d = 3$ a transition appears at $T_c = 3.9533 J/k$, whereas for $d = 1$ and $d = 2$, $T_c = 0$. For $d > 3$ a phase transition appears at a critical temperature $T_c(d)$, which is a strictly increasing function of d (see Table I).

Table I. Critical values of the temperature (T_c) and the corresponding mean potential energy per particle ($\langle v_c \rangle$) for hypercubic lattices in d dimensions

d	kT_c/J	$\langle v_c \rangle$ /J
3	3.9573	−1.0216
4	6.4537	−0.7728
5	8.6468	−0.6759
6	10.7411	−0.6283
7	12.7982	−0.6009
8	14.8334	−0.5833
9	16.8579	−0.5710

The free energy per particle, f, for vanishing field is given by:

$$-\beta f = \begin{cases} 2Kz - \frac{1}{2} - \frac{1}{2}\ln(4K) - \frac{1}{2}f_d(z) & \text{for} \quad T > T_c \\ 2dK - \frac{1}{2} - \frac{1}{2}\ln(4K) - \frac{1}{2}f_d(d) & \text{for} \quad T < T_c \end{cases} \tag{5}$$

And for nonvanishing external field:

$$-\beta f = 2Kz - \frac{1}{2} - \frac{1}{2}\ln(4K) - \frac{1}{2}f_d(z) + \frac{K(H/J)^2}{(z - \lambda_1/2)^2}. \tag{6}$$

It can be seen that the only singularity of the free energy occurs for $z_c = \lambda_1/2 = d$, in the absence of external field. Thus, the presence of a phase transition is determined by inserting this condition into the saddle point equation Eq. (3) which must then be solved for $K_c = K(z_c = d)$ in order to determine T_c. The saddle point equation can be rewritten in a more convenient form:[19,20]

$$4K = \int_0^\infty ds\, e^{-zs}[I_0(s)]^d \tag{7}$$

where $I_0(s)$ is the modified Bessel function of zero order.

As in previous works, the thermodynamic function that we will use to perform the comparison between the statistical mechanics and the topological approaches is the average potential energy per particle $\langle v \rangle$. For the spherical model, the averaging in the canonical framework yields

$$\langle v \rangle = \begin{cases} \frac{J}{4K} - Jz + \frac{H^2/4J}{z-\lambda_1/2} & \text{for} \quad H \neq 0, \forall T \\ \frac{J}{4K} - Jz & \text{for} \quad H = 0,\ T > T_c \\ \frac{J}{4K} - Jd & \text{for} \quad H = 0,\ T < T_c \end{cases} \tag{8}$$

In Table I we show some values of the critical temperature with the corresponding values of $\langle v_c \rangle$. It can be shown that $\langle v_c \rangle \to -1/2$ for large enough d.[20]

Although the specific details of the potential energy per particle depend on the dimensionality of the lattice, some features can be found that are common to all hypercubic lattices. In the limit of $T \to \infty$ the potential energy always vanishes. In the opposite limit ($T \to 0$) the potential energy falls to its smallest possible value $\langle v_0 \rangle = -d$. The phase transition in this model, when it occurs, is continuous.

4. TOPOLOGY

In the topological approach to phase transitions[3] one analyzes the topology of the submanifolds M_v looking for changes in their topology as v is increased. The PES M_v is that region of the configuration space that satisfies $V(\epsilon_1, \ldots, \epsilon_N)/N \leq v$. A topological transition happens at a certain value v_{TT} if the manifolds $M_{v_{TT}-\epsilon}$ and $M_{v_{TT}+\epsilon}$ are *not* homeomorphic[21] for arbitrarily small ϵ.

The relation between the PES and the thermodynamics of a system is not straightforward. To make a connection with statistical mechanics, Casetti *et al.* made the nontrivial ansatz that *v can be identified with $\langle V \rangle/N$, the thermodynamical average of the potential energy per particle.* Making use of this correspondence, for a general class of potentials, Franzosi et al.[13] showed that phase transitions can only happen at points where there is a topological change. Thus, this is a *necessary* but not a *sufficient* condition. Since then, several models have been studied in order to find sufficiency conditions.[5,8,9,11,12,14] Nevertheless, most of these models are mean field in nature and thus violate at least one of the conditions of the theorem of Franzosi *et al.* The spherical model considered here, while a short range one, does not obey additivity as a consequence of the spherical constraint (see the discussion in Sec. 7). We will show that it is in agreement with the implications of the theorem, but nevertheless, our results lead to the inexistence of a general sufficiency condition as pointed out above.

To study the topology of the phase space, it is most convenient to write the potential using the coordinates that diagonalize the interaction matrix through an orthogonal transformation (we set $J = 1$):

$$V = -\frac{1}{2} \sum_{i=1}^{N} \lambda_i \, x_i^2 - \sqrt{N} x_1 H \tag{9}$$

where λ_i, ($i = 1, \ldots, N$), are the eigenvalues of the interaction matrix, ordered from largest to smallest. In general, these eigenvalues will be degenerated. We define the sets C_a, $a = 0, \ldots, \hat{N}$, where $\hat{N} + 1$ is the number of *distinct* eigenvalues. C_a is the set containing the indices of the eigenvalues that have the $(a + 1)$-th largest value. Therefore, $|C_a|$ gives the degeneracy associated to the $(a + 1)$th largest eigenvalue. The Frobenius-Perron theorem ensures that the largest eigenvalue is not degenerated, i.e. $C_0 = \{1\}$.

The critical points of the potential energy function on the sphere are found using Lagrange multipliers. The critical point equations are:

$$\begin{aligned} x_1(2\mu + \lambda_1) + \sqrt{N}H &= 0 \\ x_i(2\mu + \lambda_i) &= 0, \qquad i = 2, \ldots, N \\ \sum_{j=1}^{N} x_j^2 &= N \end{aligned} \tag{10}$$

where μ is the Lagrange multiplier that results from enforcing the spherical constraint. From these equations and Eq. (9), $\hat{N} + 1$ critical solutions are obtained, whose potential energies are denoted v_a, $a = 0, \ldots, \hat{N}$ (ordered from smallest to largest). Each v_a corresponds to a different set of eigenvalues, namely $v_a = h(\lambda_j)$, with $j \in C_a$, and $h(\lambda_j) = -\lambda_j/2$ for $H = 0$, and $h(\lambda_j) = -\lambda_j/2 + H^2/2(\lambda_1 - \lambda_j)$ for finite H.

Notice that the degeneracy of the eigenvalues causes that the corresponding critical points be in fact *critical submanifolds*. This implies that in the directions tangent to the critical submanifolds the Hessian vanishes, which in turn implies that the potential is not a proper Morse function. But, using spherical coordinates, it can be shown that $V(x_1, \ldots, x_N)$ is nondegenerate in Bott's extended sense:[22] the Hessian does not vanish in the directions normal to the critical submanifolds. More precisely, the Hessian has $\sum_{b=0}^{a-1} |C_b|$ negative eigenvalues when restricted to the submanifold normal to the ath critical submanifold, i.e., at the critical energy v_a. This number is denoted the *index* of the critical submanifold. This generalizes to critical submanifolds the definition of index of a saddle point. Using this extension of Morse theory the Euler characteristic can be found exactly. However, profiting from the symmetry of the spherical model, we prefer to take a more direct route to study its topology. As we show below, for vanishing external field it is possible to characterize completely the topology of the M_v, by explicitly giving the values of *all* the Betti numbers. Notice that this is much more than what is possible within Morse theory, because from it one can only obtain the alternate sum of the Betti numbers (i.e. the Euler characteristic), or bounds for them.[10]

In the next two subsections we analyze, respectively, the cases of $H = 0$ and $H > 0$.

4.1. $H = 0$

For $H = 0$ the critical manifolds Σ_{v_a}, $a = 1, \ldots, \hat{N}$, are given by $\Sigma_{v_a} = \{\mathbf{x} \in \Gamma : \sum_{i \in C_a} x_i^2 = N\}$. These are (hyper)spheres whose dimension is given by the degeneracy of the corresponding eigenvalues.

To understand the nature of the topological change that happens at a critical value of v it is necessary to know the topology of the submanifolds M_v for values of v between two critical values. In Appendix A we show that in the interval (v_a, v_{a+1}) all the submanifolds are homotopy equivalent to $\mathbb{S}^{D_a-1}$, which is the D_a-dimensional sphere, with $D_a = \sum_{b=0}^{a} |C_b|$. It must be stressed that the submanifolds M_v are always N-dimensional,[23] and therefore they are never *identical* to $\mathbb{S}^{D_a-1}$. Homotopy equivalence implies the isomorphism of the homology groups of the manifolds compared.[24] Therefore, the Betti numbers of the manifolds M_v in the interval (v_a, v_{a+1}) are:

$$b_i(M_v) = \begin{cases} 1 & \text{for } i = 0 \text{ and } i = \sum_{b=0}^{a} |C_b| - 1 = D_a - 1 \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

This shows that at each v_a a *topological transition* occurs that changes the topology of the phase space from one homotopically equivalent to $\mathbb{S}^{D_{a-1}-1}$ to one homotopically equivalent to $\mathbb{S}^{D_a-1}$. In terms of the Betti numbers, each transition changes the Betti numbers at most from 0 to 1. Thus, at variance with what happens in other models (e.g. the XY model studied in Ref. 4), the *magnitude* of the Betti numbers is not a useful quantity to characterize the topological transition. More information is given by $D_a - 1$, the highest *index* of the Betti number that changes at each transition, i.e. the dimension of the deformation retract of the manifolds. As shown above, the increase of this number at each transition is given by the degeneracy of the corresponding eigenvalue. If the degeneracy of the eigenvalues is $o(N)$, in the $N \to \infty$ limit D_a is equivalent to the index of the critical manifolds, $\sum_{b=0}^{a-1} |C_b|$. Since the manifolds M_v are always homotopy equivalent to spheres whose dimension changes with v, the knowledge of D_a as a function of v implies the complete knowledge of the topology, up to homology.

As happens with other short range potentials, in the spherical model it can be shown that, if each spin interacts only with spins at a distance $O(\sqrt{N})$ (or smaller) in the lattice, and there is translational symmetry, the spectrum of eigenvalues is continuous in the $N \to \infty$ limit.[25] This implies that the set of $\hat{N} + 1$ critical energies, in this limit, will be dense in $[-d, d)$, the interval of allowed potential energies. As a consequence, for infinite size systems and considering that D_a is $O(N)$, it is convenient to introduce a continuous and normalized version of D_a, $d(v) = D_a/N$, and also a *degeneracy density* $c(v)$. They are related by $c(v) = \frac{\partial d(v)}{\partial v}$. In the following we concentrate on the properties of these quantities.

We specialize to the case of cubic lattices in d dimensions where the spins interact isotropically only with their first $2d$ neighbours. In principle, this analysis can be extended to any other short range version, with the conditions mentioned above.

The spectrum of the adjacency matrix of the lattice is given by:

$$\lambda(\mathbf{p}) = 2 \sum_{i=1}^{d} \cos(2\pi p_i / N^{1/d}), \qquad p_i = 0, \ldots, N^{1/d} - 1 \tag{12}$$

Because of the translational symmetry of the potential, each eigenvalue is at least 2^d-fold degenerate. The degeneracy density $c(v)$, in the infinite size limit, is given by:

$$\frac{1}{N}\sum_{\mathbf{p}} \delta_{\lambda(\mathbf{p}),-2v} \quad \overset{N\to\infty}{\longrightarrow}$$

$$\begin{aligned} c(v) &= \int_0^{2\pi} \left(\Pi_{i=1}^{d} \frac{d\omega_i}{2\pi}\right) \delta(v + \lambda(\omega)/2) \\ &= \int_0^{\infty} \frac{dx}{\pi} \cos(x\, v)(J_0(x))^d \end{aligned} \tag{13}$$

where the delta functions in the first and second lines are a Kronecker and Dirac one, respectively, $\lambda(\omega) = 2\sum_{i=1}^{d} \cos(\omega_i)$, and $J_0(x)$ is the Bessel function of zeroth order (in Fig. 1 we plot $c(v)$ and $d(v)$ for $d = 2$, $d = 3$ and $d = 4$). In the Appendix B we show that the integral converges uniformly for all values of d and therefore $c(v)$ is a continuous function. The derivatives with respect to v can be obtained by performing the derivative inside the integral. But, as this is only valid if the resulting integral converges, this procedure allows us to obtain only the first $\lfloor (d-1)/2 \rfloor$ derivatives. But this will be enough for our purposes. In the appendix we show that all these derivatives are continuous, except for the last, which is discontinuous *only* at the following points: at odd values of v if d is odd, at values of v such that $v/2$ is even if $d/2$ is odd and such that $v/2$ is odd if $d/2$ is even. But these values are clearly different from the ones at which a thermodynamical phase transition takes place, for all values of d (see Table I). Note that, trivially, the manifolds M_v display TTs at the points $\langle v_c \rangle$ where PTs occur, since there is a continuum of TTs. Most of these TTs, however, are *not* particularly abrupt or strong. And those that can be considered abrupt do not coincide in its value with the PTs, as we have shown above. This proves that up to the $\lfloor (d-1)/2 \rfloor$ derivative there is no particular correlation between TTs and PTs.

The only possibility left to look for a relationship between topological transitions (in the sense of a discontinuity of some function of the topology of the potential) and thermodynamical phase transitions would be in the higher derivatives of $c(v)$, which cannot be studied by exchanging the integral and derivative operations. This possibility seems to us rather unreasonable, because it would imply not only that the derivative where discontinuities are to be looked for depends on the dimension of the lattice, but also that those discontinuities present in earlier derivatives should be disregarded.

We have thus shown that discontinuities in the derivative of $c(v)$ are not sufficient to induce a PT. Furthermore, we will show in the following that, even though in the case of a nonzero external field there appear discontinuities in the

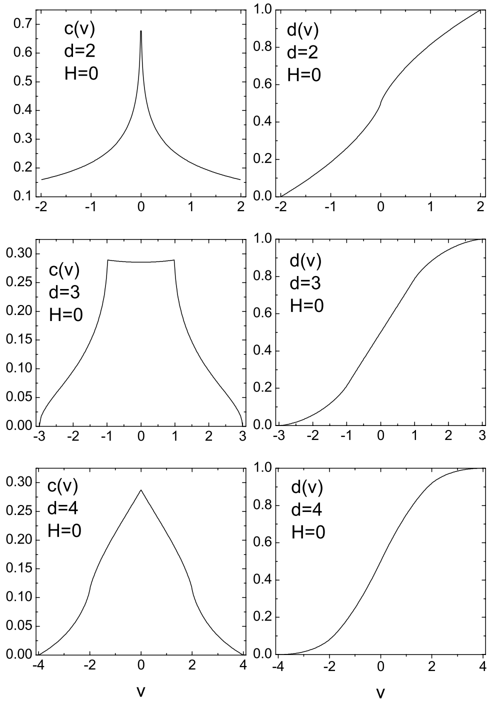

Fig. 1. Degeneracy density $c(v)$ and relative index $d(v)$ of the critical manifolds, for a vanishing external field.

function $c(v)$ *itself*, no connection between such TTs and PTs can exist, simply because the model does not display any PTs at all.

4.2. $H \neq 0$

In the case of nonvanishing field it is not so easy to find the homotopy type of the submanifolds M_v, because of the break of the symmetry introduced by the external field term in the hamiltonian. Nevertheless, using Morse theory it is at least possible to establish the homotopy type of the submanifolds up to above the second smallest critical energy, where an abrupt topological change is shown to take place.

According to Morse theory, the manifolds M_v of a smooth function are homeomorphic for all $v \in (a, b)$ if there are no critical points in this interval. If there is one critical point at $c \in (a, b)$, the manifold $M_{c+\epsilon}$ is homeomorphic to $M_{c-\epsilon} \cup e_k$, where e_k is a k-cell. In other words, at the critical point a k-cell (i.e. a k-dimensional open disk) is attached to the manifold. k is the *index* of the critical point, defined as the number of negative eigenvalues of the Hessian at that point.

Returning to the critical point equations (10), with λ_i given by (12), from the solutions $x_1 \neq 0, x_i = 0, \forall i > 1$ we get two critical values of the potential energy function. The first one, $v_+ = -(\lambda_1/2 + H)$ is the smallest critical energy, corresponding to the critical point $\mathbf{x}_+ = (-\sqrt{N}, 0, \ldots, 0)$ $(H > 0)$. The second smallest critical value, $v_- = -(\lambda_1/2 - H)$, corresponds to the critical solution $\mathbf{x}_- = (+\sqrt{N}, 0, \ldots, 0)$. Other solutions, with $x_i \neq 0$ for some values of $i > 1$, arise at critical values $v_a = -\lambda_k/2 + H^2/2(\lambda_1 - \lambda_k)$, where $k \in C_a$, $a \geq 2$. The corresponding critical point solutions only lie on the sphere $\mathbb{S}^{N-1}$ for k such that $\lambda_1 - \lambda_k > H$. Notice that there is a threshold energy v_{th} above which the levels have been shifted by an amount $H^2/2(\lambda_1 - \lambda_k)$ – with respect to the case of vanishing H – and below which the critical values have been supressed (i.e. they are no longer critical).

The Hessian, calculated on the spherical surface $\mathbb{S}^{N-1}$ at the critical points $\mathbf{x}_\pm$ is a diagonal matrix whose eigenvalues are $V_{ii}^\pm = \lambda_1 \pm H - \lambda_i$. Therefore, at these two points the Hessian is not singular (except for some particular values of H), which implies that $\mathbf{x}_\pm$ are non-degenerate critical points. Since λ_1 is the largest eigenvalue, for v_+ all V_{ii}^+ are positive. This was to be expected because $\mathbf{x}_+$ is the absolute minimum of the potential. Topologically this means that for $v_+ < v < v_-$, M_v is homotopically equivalent to a disk, i.e. to the 0-cell attached to the empty manifold at v_+.

As for the nature of the critical point $\mathbf{x}_-$ at v_-, it depends on the field strength. If H is such that the second largest eigenvalue $\lambda_k \in C_2$ obeys $\lambda_k < \lambda_1 - H$, then $\mathbf{x}_-$ is also a minimum. Thus, if v_2 is the next critical value, for $v \in (v_-, v_2)$, M_v is homotopically equivalent to the union of two disks. We have shown, however, that for large values of N the spectrum of the adjacency matrix becomes dense, which implies that a certain number $n = \max\{k : \lambda_k > \lambda_1 - H\}$ of its eigenvalues will not obey the above inequality. The critical energies constructed from these eigenvalues, $v_a = -\lambda_k/2 + H^2/2(\lambda_1 - \lambda_k)$, $k \leq n$, will fall in the interval (v_+, v_-). However these energies are not critical values, since the corresponding critical point solutions do not lie on the sphere $\mathbb{S}^{N-1}$. From the expression for V_{ii}^-, we see that n is just the index of the critical point $\mathbf{x}_-$, which gives the dimension of the cell that is attached to the disk at v_-. It can be proved[21] that the result of this attachment is homotopy equivalent to the attachment of the same cell to a point. The manifold M_v for $v \in (v_-, v_2)$ is therefore homotopically equivalent to a sphere of n dimensions, which is the only possible result of the attachment. Notice that for large values of N, n becomes macroscopic, i.e. proportional to N. We then see that in the interval (v_+, v_-) there are no topological changes in the manifolds M_v, which have the homotopy type of a point, and that at v_- an abrupt change in the topology takes place: the manifold has then the homotopy type of a sphere with a macroscopic number of dimensions (see the jump of $c(v)$ in Fig. 2).

The critical point solutions arising at the critical energies $v_a > v_-$ are degenerated, as a consequence of the degeneracy of the eigenvalues of the adjacency

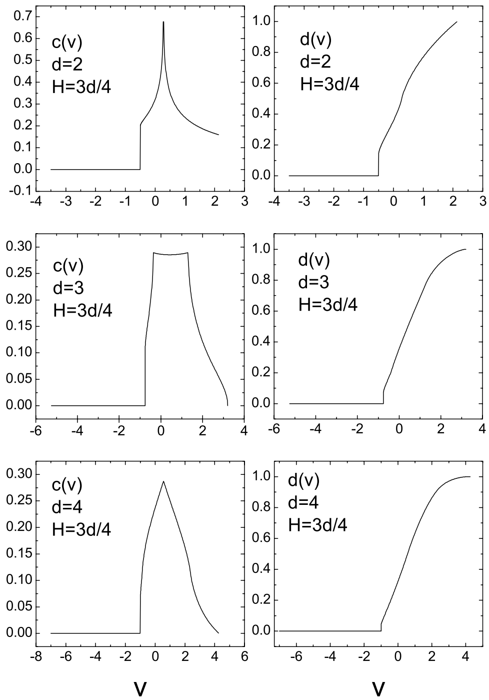

Fig. 2. Degeneracy density $c(v)$ and relative index $d(v)$ of the critical manifolds, for a finite field. A delta function is assumed at the discontinuity point in the graphs of the left column.

matrix. It is possible to calculate the indexes of these critical submanifolds, which turn out to be identical to the case of vanishing field. Since the function $v_a(\lambda_k)$ is a monotonously increasing function for decreasing eigenvalues, the index of the critical submanifolds as a function of v, $d(v)$, starting from v_{th}, is the same function as in the case of $H = 0$ (see Fig. 2).

The main difference with the results in the previous section is that in this case the connection between the index and the topology of the M_v is less obvious. We have not been able to identify the homotopy types for all values of v. Using Bott's extension of Morse theory[22] it is possible to determine the submanifolds that are attached at each critical point from $d(v)$. But this is not sufficient to determine the homotopy type of the manifolds M_v.

Nevertheless we have been able to find exactly the topological change that takes place at v_-, and have shown that it is *macroscopic*. It may come as a surprise that this very abrupt change in topology has no correspondence with a thermodynamical phase transition.

5. ENSEMBLE EQUIVALENCE

The results from the topological analysis are to be compared to the *a priori* known thermodynamical behavior of the system. In systems for which ensemble equivalence does not hold, ambiguity arises, as to which ensemble's behavior the topological outcome should be compared to. Recently, M. Kastner[6] found that for the mean field spherical model, the microcanonical and canonical ensembles are only partially equivalent. While in the latter ensemble a continuous PT occurs, the former one displays no PT, and the thermodynamics of both ensembles coincide in the low energy phase. This finding put in a new perspective the conclusions of Ref. 14 about the topological mechanism for phase transitions. This is why, in this section, the microcanonical thermodynamics of the Berlin and Kac spherical model is further discussed. It is a known fact that ensemble equivalence is guaranteed as long as the interactions decay rapidly enough with distance. Although we are dealing here with the spherical model with nearest neighbor interactions, the presence of the spherical constraint *might* play – in the thermodynamic limit – the role of an infinite ranged interaction. Although the canonical PTs have been shown to be uncorrelated to the discontinuities in the derivatives of $c(v)$, we could expect the results from topology to lead to a different interpretation when compared to microcanonical thermodynamics, in case the two ensembles do not coincide.

Behringer[26] already demonstrated ensemble equivalence in the model by showing that the canonical and microcanonical critical exponents obey the appropriate relation (in this system, they coincide), and that the microcanonical PTs exist for the same lattice dimensions as the canonical PTs. We, alternatively, verify ensemble equivalence using the criterion defined in Ref. 27, by showing that the microcanonical entropy and Legendre transform of the canonical free energy, $s(v)$ and $s^{**}(v)$ respectively, coincide in their entire domains of definition and, furthermore, that the first derivative $\beta = \partial s(v)/\partial v$ spans the whole interval $[0, +\infty)$.

The starting point for the microcanonical thermodynamics computation is the density of states

$$\Omega_N(v, H) = A_N^{-1} \int \dots \int_\Gamma d\epsilon_1, \dots, d\epsilon_N \; \delta[V(\epsilon) - Nv], \tag{14}$$

where $V(\epsilon)$ is given by Eq. (1).

After some algebra, analogous to the one carried out in Ref. 16 for the canonical ensemble we arrive at

$$\Omega_N(v, H) \propto \int_{-i\infty}^{+i\infty} d\mu \int_{\alpha-i\infty}^{\alpha+i\infty} d\eta \; e^{N\bar{s}_N(\mu,\eta;v,H)}, \tag{15}$$

where we have defined $\bar{s}_N(\mu, \eta; v, H) \equiv \mu v + \eta - \mu^2 H^2 \left[4(\mu d - \eta)\right]^{-1} - f_N(\mu, \eta)$ and $f_N(\mu, \eta) \equiv \frac{1}{2N} \sum_{\mathbf{p}} \ln(-\frac{\mu}{2}\lambda(\mathbf{p}) + \eta)$.

In the limit $N \to \infty$, we have $f(\mu, \eta) = \frac{1}{2} \frac{1}{(2\pi)^d} \int \ldots \int_0^{2\pi} d\omega_1, \ldots, d\omega_d \ln(-\mu \sum_{l=1}^{d} \cos \omega_l + \eta)$.

Applying the saddle point method, the density of states is given by

$$\Omega_N(v, H) \approx \frac{\pi^{N/2} \; e^{N\bar{s}_N(\mu_s, \eta_s; v, H)}}{\pi \sqrt{N} A_N[(\bar{s}_N)_{\eta\eta}(\bar{s}_N)_{\mu\mu}]^{1/2}}, \tag{16}$$

where the saddle point (μ_s, η_s) is solution of the equations $\partial \bar{s}_N/\partial \mu = 0$ and $\partial \bar{s}_N/\partial \eta = 0$, and $(\bar{s}_N)_{\eta\eta} > 0$ and $(\bar{s}_N)_{\mu\mu} > 0$ are the second derivatives of the function calculated at the saddle point. Considering η and μ over the real axis, with $\mu \in [-\eta/d, \eta/d]$ and $\eta > 0$, $\bar{s}_N \to \infty$ whenever $\mu \to \pm\eta/d$. Thus, $|\bar{s}_N|$ has at least one minimum over the real axis. Moreover, $(\bar{s}_N)_{\mu\mu}$ and $(\bar{s}_N)_{\eta\eta}$ for real μ and η are non-negative, which means that this minimum is unique.

Defining $x \equiv \eta/\mu$ (in this case, we choose real $x \in [d, \infty)$), it is possible to reduce the two-dimensional saddle point system of equations to a one-dimensional one[29]

$$\left[v + x - \frac{1}{A_0(x)}\right] - H^2 \left[\frac{1}{4(d - x)} - \frac{1}{4(d - x)^2} \frac{1}{A_0(x)}\right] = 0, \tag{17}$$

where $A_0(x) \equiv \frac{1}{(2\pi)^d} \int \frac{d^d\omega}{x - \sum_{l=1}^{d} \cos \omega_l} = \int_0^{\infty} dt \; e^{-xt} \; (I_0(t))^d$.[28] Moreover, from the original saddle point equations we get $\mu_s = 2(d - x)/[4(v + x)(d - x) - H^2]$.

For $d \geq 3$, the integral A_0 remains finite at $x = d$. For $d = 1, 2$ and at $x = d$, the integral diverges.

Including the constant prefactors coming from Ω_N, and substituting for μ_s as a function of x, v and H, we get, for the entropy density $s = \lim_{N\to\infty} \frac{1}{N} \ln \Omega_N(v, H) = -1/2 - \ln(2)/2 + \bar{s}$, which may also be expressed as a function of x alone

$$\begin{aligned} s(v, H) = \frac{1}{2} \ln \left[(v + x(v, H)) - \frac{H^2}{4(d - x(v, H))}\right] \\ - \frac{1}{2(2\pi)^d} \int d^d\omega \ln \left[x(v, H) - \sum_{l=1}^{d} \cos \omega_l\right], \end{aligned} \tag{18}$$

where $x(v, H)$ is the solution x of Eq. (17).

From the second term of $s(v, H)$, we see that as $x \to d^+$, the system approaches a non-analyticity point of the integral. Thus, the occurrence or not of a phase transition will be determined by the behavior of the integral A_0 at $x = d$.

First we fix $H = 0$. For $d = 1, 2$, as mentioned before, A_0 diverges, which implies $v_c = -d$. Thus, the ferromagnetic phase can only arise at the ground state.

For $d \geq 3$, however, the critical values v_c are clearly above $-d$:

$$v_c = \frac{1}{\int_0^\infty dt\,[e^{-t} I_0(t)]^d} - d. \tag{19}$$

These values do indeed coincide with the critical energies from the canonical ensemble. For finite field, as $x \to d^+$, since $A_0 > 0$, the expression that multiplies H^2 in Eq. (17) diverges. Thus, for $H \neq 0$, the saddle point solution $x = d$ never exists, and consequently, no phase transition occurs for any d.

If we compute the equation of state of the system (as in Ref. 26)

$$m = \frac{1}{\beta}\left(\frac{\partial s(v, H)}{\partial H}\right)_v = \left(\frac{\partial s(v, H)}{\partial v}\right)_H^{-1}\left(\frac{\partial s(v, H)}{\partial H}\right)_v, \tag{20}$$

we find, for small fields:

$$m(x(v, H) - d) \approx H/2. \tag{21}$$

Hence we see that the spontaneous magnetization, when $H = 0$, is only nonzero if $x(v, 0) = d$ through the ferromagnetic phase. This result expresses the “sticking” of the saddle-point below the transition, which is also observed in the canonical computation.[16]

To verify ensemble equivalence, we should be able to show that[27]

$$s^{**}(v, H) \equiv \inf_\beta \{\beta v - \beta f(\beta, H)\} = s(v, H), \tag{22}$$

where $f(\beta, H)$ is the Gibbs free energy computed through the partition function.[16] In other words, that the Fenchel-Legendre transform of $f(\beta, H)$ coincides with $s(v, H)$.

From the canonical results obtained in Ref. 16, we have Eqs. (5) and (6) for the Helmholtz free energy per particle. The (canonical) saddle point equation is just Eq. (3), recalling that $K = \beta J/2$.

It is clear that $df_d(z)/dz = A_0(z)$. The equation defining $\bar{\beta}(v, H)$, which minimizes $(\beta v - \beta f(\beta, H))$, is

$$2\bar{\beta}(v + z_s(\bar{\beta})) = 1 - \frac{H^2\bar{\beta}}{2(z_s - d)}. \tag{23}$$

Substituting into $s^{**}(v, H)$, and using the saddle point Eq. (3) in the definition of $\bar{\beta}(v, H)$, we see that $x(v, H)$ defined by (17) coincides with $z_s[\bar{\beta}(v, H)]$, and we reobtain $s(v, H)$ of Eq. (18).

The critical energies (19) turn out to be negative. Furthermore, in contrast to what happens in the mean field case, as $v \to 0$, $\beta \to 0-$ and, evidently, as $v \to -d$, $\beta \to \infty -$, which means that in this case the paramagnetic phase is accessible.

Hence, together with the fact that $s(v) = s^{**}(v)$ for all $v \in [-d, 0)$, the fact that $\partial s/\partial v$ assumes all values in $[0, \infty)$, shows that *complete* ensemble equivalence holds. Contrary to the MF case,[6] there is no ambiguity in the consequences implied by the topological results of the previous section.

6. LONG RANGE CONNECTIONS

In Ref. 14 the case of a fully connected system was studied, which corresponds to a mean field approach. This case is very different from the short range model: the interaction matrix has only two distinct eigenvalues, N and 0, the latter with multiplicity $N - 1$. The topological scenario is then a very simple one. There are only two TTs, one at the minimal potential energy and the other at the maximum. This last one corresponds to a thermodynamic phase transition (in the canonical ensemble) taking place at $\beta_c J = 1$.

To probe a bit further the concept of the sufficiency condition for a TT to be able to induce a PT, it is interesting to study what happens when the connections are long ranged but do not span the whole lattice. To be specific, we consider the following two cases.

In the first case each spin interacts with its closest aN neighbors ($a < 1$). As the number of connections of each spin is proportional to N, the potential energy must be rescaled accordingly (by dividing it by N) to obtain meaningful results. This entails a rescaling of the eigenvalues of the adjacency matrix. The matrix for a d-dimensional lattice is a circulant block matrix where each block is the (circulant) adjacency matrix of a suitable $d - 1$ dimensional lattice. Its eigenvalues can be recursively calculated using simple properties of circulant matrices. In the infinite N limit we get

$$\lambda_{p_1,\ldots,p_d}(a) = \frac{1}{\pi^d} \sum_{i=1}^{d} \frac{p_i^{d-2} g_d(2\pi a^{1/d} p_i)}{\prod_{k\neq i}^{d}(p_i^2 - p_k^2)} \quad \text{for } d \geq 2$$

$$\lambda_p(a) = \frac{1}{\pi} \frac{\sin(2\pi a\, p)}{p} \qquad \text{for } d = 1 \tag{24}$$

where $p_i = 1, \ldots, N^{1/d}$ for all i and $g_d(x) = (-1)^{d/2}\cos(x)$ if d is even and $g_d(x) = (-1)^{(d-1)/2}\sin(x)$ if d is odd.

In the second case each spin interacts with all the hypercube of side $2aN$ that has it as center (extended Moore neighbourhood), the eigenvalues of the connection matrix are $\lambda_{p_1,\ldots,p_d} = \prod_{i=1}^{d} \lambda_{p_i}(a^{1/d})$, where $\lambda_{p_i} = \lambda_p$, given by Eq. (24).

Thus, similarly to what happens for the short range model discussed before, in these cases there is an infinity of values of v at which TTs occur. The main difference now is that the spectrum is discrete. As it is unreasonable to postulate the existence of an infinity of PTs one should look for some special feature of the spectrum that can be associated to a PT. One such feature is an accumulation point. It is easy to see that the mentioned models have only one accumulation point, occurring at $\lambda = 0$.

Because of the discreteness of the spectrum and the accumulation point at $\lambda = 0$, the thermodynamics of these models turns out to be remarkably simple. The function $f_d(z)$ (see Eq. (4)) can be readily calculated and it gives, for all dimensions in both models, $f_d(z) = \ln(z)$ in the thermodynamic limit, as in the fully connected model. Using the fact that the critical saddle point $z_c = a/2$, and replacing this in Eq. (3) we obtain that the critical temperature of the PT is $\beta_c = a/J$. This corresponds to $v = 0$, as in the fully connected model.[14] This is not a coincidence: using the same reasoning it can be shown that, if the connection matrix had a discrete spectrum with an accumulation point at some value $\lambda < a/2$ (and therefore $f_d(z) = \ln(z - \lambda)$), the PT would occur at exactly $v = J\lambda$ (and $\beta_c = (a - 2\lambda)/J$).

When a field is turned on, the situation is also the same as for the fully connected model: no PT appears and the TT is in a place of configuration space that cannot be thermodynamically reached by the system.

7. CONCLUSIONS

We have characterized exactly the homology of the successive manifolds of configuration space of the short range spherical model. We have shown that even though there is a continuum of topological transitions, a function of the topology — which completely characterizes it — can be defined for which some discontinuities in the function itself ($H \neq 0$) or in its derivatives are found at specific v points. However, they are not coincident with the phase transitions which occur for vanishing external field. The topological transitions which do happen at the PT points are 'smooth,' and do not display any particular distinguishing feature. If these TTs were to be related to the origin of the corresponding PTs, we could not expect them to be the *only* active mechanism. Moreover, the occurrence of the above mentioned discontinuities, which do represent abrupt topological transitions, having no relation to any PT, challenges the expectation that a topological transition in the M_v's may have any relevant role in the origin of the phase transition. Hence, the topological approach does not apply to this model.

The proof that for short-range, confining, stable potentials, a topological transition *must* take place at the point of the phase transition,[13] implies that topology ought to play *some* role in this event, at least for this class of potentials. So far, the models where topological hypothesis applies do not satisfy at least one of the conditions of the theorem, and thus do not fall into this class. On the other hand, among the models that were found to violate the topological hypothesis, none fulfills all the conditions of the theorem. In particular, except for the model analyzed in Sec. 4, none is short ranged. For topological transitions to be defined as a possible *sufficient* mechanism to originate a PT, it would be necessary to establish a class of potentials to which it applies, and a sufficiency condition on the type and/or 'strength' of the topological transitions involved. Such results are still lacking. Although the spherical model we study here is short ranged, confining and bounded below, it might not satisfy one of the conditions of the theorem. This is the condition that the potential be *additive*, which essentially says that for a system of $2N$ spins this potential should satisfy $V(2N) \to V(N) + V(N)$ in the infinite N limit. Now it is not clear how to define additivity in presence of the spherical constraint. Whether or not the spherical model is excluded by the requirements of the theorem, its implications are not significant for this model, because in the $N \to \infty$ limit we have a continuum of TTs, and therefore the simple existence of topological transitions is not enough to predict phase transitions. Hence, the role played by topology in the phase transition seems irrelevant in this case. To look for the effect of the PES topology on the phase transition of a model fulfilling *all* the requirements of the theorem would be a very elucidative contribution to the field. As far as we know, the short range spherical model is, among the models already studied, the closest one to this class of potentials.

The increasing number of models for which the topological mechanism seems to be at least insufficient, and moreover, in some cases, completely decorrelated from the occurrence of phase transitions, puts in doubt the possibility of an origin of these phenomena at the level of microscopic interactions (in the sense exploited in the Introduction of this paper). In particular, in view of the latest negative results on the TH, recent works on the ϕ^4 mean field model[(30,31)] have led to the proposal of alternative mechanisms as responsible for the triggering of a phase transition. Hahn and Kastner found that the nonanalyticity in the microcanonical entropy density function of the ϕ^4 MF model arises only as a consequence of its maximization with respect to the magnetization. This is a totally distinct mechanism from the topological one, since the topological approach suggests that the possible origin of PTs could be found before the definition of statistical ensembles. This mechanism is relevant, in particular, for the characterization of phase transitions within the microcanonical ensemble.

This maximization mechanism, however, is only possible for long range interactions, and thus certainly does not apply to the short range spherical model. Within this perspective, one should search for *at least* a third mechanism responsible for the PTs in the model here studied. Moreover, in the case of non-confining potentials, yet another possible 'singularity-generating' mechanism has been pointed out, namely, the loss of compactness of the manifolds Σ_v or M_v. But this multiplicity of very distinct mechanisms seems to undermine the appealing and pretended universality of the original topological hypothesis.

The topological properties of the PES are known to have important effects on the *dynamics* of systems with and without disorder (see e.g. Refs. 32 and 33). Indeed, the dynamical transition in the p-spin spherical spin glass, for example, is known to be related to the vanishing of the order of the saddles in the PES at a given value of the energy.[34] A similar topological mechanism is at work at the mode coupling dynamical singularity in structural glasses.[35,36] Several dynamical properties at the dynamical singularity are related to the occurrence of zero eigenvalues of the hessian of the potential energy (flat directions on the PES).[32–34] Since the first proposal of the topological approach it has been advanced that it might serve as a unifying formalism for the diverse kinds of phase transitions, including dynamical PTs. This possibility, as far as we know, has not yet been explored in any of the models that display a dynamical PT.

With regard to the spherical model studied in this paper, one intriguing question that arises is whether the topologically abrupt changes that we have found, in particular the discontinuity in the functions $d(v)$ and $c(v)$ in the case of nonvanishing field, can have any influence on the *dynamics* of the model.

APPENDIX A: DEFORMATION RETRACTION OF M_v FOR $H = 0$

In this section we show that M_v is homotopically equivalent to $\mathbb{S}^{D-1}$, where $D = \max\{k : \lambda_k > -2v\}$. In fact we prove that $\mathbb{S}^{D-1}$ is a deformation retract of M_v, which in turn implies their homotopy equivalence.[21]

A submanifold S is a deformation retract of a manifold M if there exists a series of maps $f^\nu : M \to M$ with $\nu \in [0, 1]$, such that $f^0 = I$, $f^1(M) = S$ and $f^\nu|_S = I$ for all ν. The map when considered as $f : M \times [0, 1] \to M$ must be continuous.

Let us take $v \in (v_a, v_{a+1})$, where $v_a = -\lambda_k/2,\ k \in C_a$. The deformation retraction that takes the manifold M_v onto its submanifold $\mathbb{S}^{D-1}$ is given by $\mathbf{x}(\nu) = (f_1^\nu(\mathbf{x}), \ldots, f_N^\nu(\mathbf{x}))$ with

$$f_i^\nu(\mathbf{x}) = \begin{cases} x_i\sqrt{1 + \nu \sum_{k=D+1}^{N} x_k^2 / \sum_{k=1}^{D} x_k^2} & \text{for } i \leq D \\ x_i\sqrt{1-\nu} & \text{for } i > D \end{cases} \tag{25}$$

The properties for $\nu = 0$ and $\nu = 1$ are evidently fulfilled. It can also be seen that no points are mapped outside M_v. It is easy to see that the image points always lie on the sphere $\mathbb{S}^{N-1}$, but it must also be checked that their potential energy does not exceed v. For this, let us define a trajectory as the set of points resulting of applying all the maps f^ν to a single point in M_v. The potential energy of the points in the trajectory, $V^\nu(\mathbf{x}) = V(\mathbf{x}(\nu))$ is a linear function of ν. Thus, it must be bounded by the potential energy of the endpoints. The initial point, $\nu = 0$ has $V(\mathbf{x}) < v$ by definition. The final point is on the sphere $\mathbb{S}^{D-1}$, where

$$\frac{V(\mathbf{x} \in \mathbb{S}^{D-1})}{N} = \sum_{k=1}^{D} \frac{-\lambda_k}{2} \frac{x_k^2}{N} < \sum_{k=1}^{D} v \frac{x_k^2}{N} = v \tag{26}$$

using the definition of v. We have used the fact that the trajectory is continuous, which depends on the continuity of the map, which can be readily checked. Indeed, Eq. (25) implies that the map can only be discontinuous in points $\mathbf{x}_d$ such that $x_i = 0$ for $i \le D$, but this point satisfy

$$\frac{V(\mathbf{x}_d)}{N} = \sum_{k=D+1}^{N} \frac{-\lambda_k}{2} \frac{x_k^2}{N} \ge \sum_{k=D+1}^{N} v \frac{x_k^2}{N} = v \tag{27}$$

and thus they are outside M_v.

APPENDIX B: UNIFORM CONVERGENCE

The Bessel function of order 0 can be written as Ref. 37:

$$J_0(x) = \sqrt{\frac{2}{\pi x}} \{\cos(x - \pi/4) + f(x)\} \tag{28}$$

for $x > 0$, where $f(x)$ satisfies $|f(x)| \le (2x)^{-1}$. We want to study the convergence of the k-th derivatives of $c(v)$ (Eq. (13)) for all values of k, i.e., of the functions

$$g_k(v) = \left| \int_0^\infty dx\, x^k f_k(xv)[J_0(x)]^d \right| \tag{29}$$

where $f_k(xv) = \sin(xv)$ for odd k and $f_k(xv) = \cos(xv)$ for even k. Because the integrand is continuous everywhere and in particular in the neighbourhood of 0, the convergence of the integral with $r > 0$ as lower limit implies the convergence of the one in Eq. (29).

Using Eq. (28), we get

$$\int_r^\infty dx\, x^k f_k(xv)[J_0(x)]^d$$
$$\propto \sum_{i=0}^{d} \binom{d}{i} \int_r^\infty dx\, x^{k-d/2} f_k(x\, v)(\cos(x - \pi/4))^{d-i}(f(x))^i \tag{30}$$

The bounds on $f(x)$ imply that this expression converges (uniformly) if the term with $i = 0$ converges uniformly, which happens for k smaller than $d/2 - 1$, for all values of v. Therefore, the derivatives of $c(v)$ up to the order $k = \lfloor d/2 - 1 \rfloor$ can be taken inside the integral and the resulting function is continuous.[38] For $k > d/2$ Eq. (30) diverges and therefore the derivative must be calculated by a different method (this does not imply that these derivatives diverge).

For $d/2 - 1 \le k < d/2$ a finer analysis must be performed. Again, only the first integral in the summation must be studied, because the rest of them converge uniformly. Using elementary properties of the trigonometric functions we obtain,

$$
\begin{aligned}
&\int_0^{\infty} \frac{dx}{\hat{g}_d(x)} f_k(vx)\,[\cos(x-\pi/4)]^d \\
&= 2^{-d-1}\sum_{j=0}^{d}\binom{d}{j}\int_0^{\infty}\frac{dx}{\hat{g}_d(x)}\left\{ f_k\left[(d-2j)\frac{\pi}{4}\right]\right. \\
&\quad \times [\cos((d-2j-v)x)+(-)^k\cos((d-2j+v)x)] \\
&\quad + f_{k+1}[(d-2j)\frac{\pi}{4}]\times[\sin((d-2j+v)x) \\
&\quad \left. + \ (-)^k\sin((d-2j-v)x)]\right\}
\end{aligned} \tag{31}
$$

where $\hat{g}_d(x) = x$ for even d and $\hat{g}_d(x) = \sqrt{x}$ for odd d. When none of the arguments of the cosines inside the brackets vanishes identically, the integrals converge uniformly[38] (they are, in fact, Fresnel integrals). But for some integer values of v there is in the sum one term that diverges, because the corresponding integrand is $1/\hat{g}_d(x)$. These values are: odd v if d is odd, even $v/2$ if $d/2$ is odd, and odd $v/2$ if $d/2$ is even.

This shows that up to $k < d/2 - 1$ the derivatives can be obtained by taking derivatives inside the integral and they are continuous in $v \in [-d, d]$. For $k = \lceil d/2 - 1 \rceil$ the derivative obtained has some discontinuity points where it diverges.

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