Role of saddles in topologically driven phase transitions: The case of the *d*-dimensional spherical model

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Analyzing the *d*-dimensional spherical model, we show that underlying saddles, defined through a map in the configuration space, play a central role in driving the phase transition. At the phase transition point the underlying saddle energy reaches its lowest value, corresponding to the trivial boundary topological singularity.

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I. INTRODUCTION

Since the pioneering works of Pettini and co-workers [1] (for a review, see Refs. [2,3] and references therein), many papers have been devoted to investigating the hypothesized relationship between phase transitions and topological changes in configuration space for interacting systems (*topological hypothesis*) [4–12]. The matter has been partially clarified with the demonstration of a theorem [13–15] that states that a topological change is a necessary condition for the presence of a phase transition. Specifically, this theorem asserts that the thermodynamic phase transition energy e_c corresponds to a topological change of the submanifold $M_e = \{ q | V(q) \leq Ne \}$ [q are the generalized coordinates, $V(q)$ the potential energy function, and N the number of degrees of freedom] exactly at the transition energy e_c. The theorem strictly holds for systems with a smooth, confining, bounded, and finite-range interaction potential. For a wider class of interaction potentials such a relation has not yet been established; there are model systems (mainly with mean-field interaction potentials, so not satisfying the theorem hypotheses) for which phase transitions and topological changes seem not to be strictly related. Among other examples, such a discrepancy has been recently [16] observed in the finite-dimensional spherical model [17], for which the phase transition energy has been shown not to correspond to topological changes (at least "strong" topological changes, those supposed to be related to phase transitions [3,5]).

Following previous works [18–20], we suggest the possibility that the relevant information driving the phase transition is encoded in the *underlying* saddles, i.e., the closest stationary points to explored configurations (*weak topological hypothesis*). Applying such an analysis to the spherical model [17], we find that, at the phase transition, the energy of the underlying saddles reaches the minimum value, corresponding to the trivial boundary topological singularity. Therefore, also the *d*-dimensional spherical model, similarly to other models [18,19], suggests the correctness of the topological hypothesis (even though in the weak form).

The paper is organized as follows. In Sec. II we will introduce the model, Sec. III is devoted to the thermodynamics and Sec. IV to the topological properties. The main result is presented in Sec. V, where the underlying saddle properties are investigated. Conclusions are drawn in Sec. VI.

II. THE MODEL

The *d*-dimensional spherical model is defined by N real variables ε_i lying in a *d*-dimensional hypercubic lattice, subject to the spherical constraint

$$\sum_{i=1}^{N} \varepsilon_i^2 = N, \tag{1}$$

and interacting through the Hamiltonian

$$H = -\frac{J_0}{2} \sum_{\langle i,j \rangle} \varepsilon_i \varepsilon_j, \tag{2}$$

where the sum $\langle i,j \rangle$ is over nearest-neighbors (counting twice a given pair). It is worth noting that the spherical constraint Eq. (1) introduces a sort of long-range interaction, so, strictly speaking, the model cannot be properly defined as shortranged. Diagonalizing the interaction matrix J_{ij}—which is J_0 if (i,j) are nearest neighbors, and 0 otherwise (periodic boundary conditions are applied)—the Hamiltonian can be written as

$$H = -\frac{J_0}{2} \sum_{i=1}^{N} \lambda_i x_i^2, \tag{3}$$

where $J_0 \lambda_i$ are the eigenvalues of J_{ij} and x_i are the new constrained variables, with $\Sigma_{i=1}^{N} x_i^2 = N$. The eigenvalues λ_i can be written as [16,17]

$$\lambda_{\{p_i\}} = 2 \sum_{i=1}^{d} \cos(2\pi p_i / L), \tag{4}$$

where $L = N^{1/d}$ and $p_i = 0, \ldots, L-1$. Taking into account possible degeneracy of eigenvalues, we can group together variables corresponding to the same value $\hat{\lambda}_i$, obtaining

$$H = -\frac{J_0}{2} \sum_{i=0}^{\hat{N}} \hat{\lambda}_i r_i^2, \tag{5}$$

where $r_i^2 = \Sigma_{j \in \mathcal{C}_i} x_j^2$ ($\Sigma_i r_i^2 = N$), $\mathcal{C}_i$ is the set of d_i indices with the same $\hat{\lambda}_i$ ($\Sigma_i d_i = N$), and $\hat{N}+1$ is the number of distinct eigenvalues $\hat{\lambda}_i$.

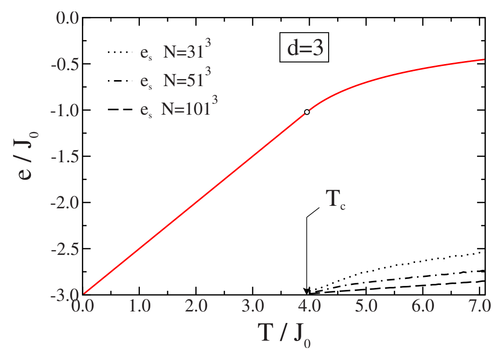

FIG. 1. (Color online) Energy as a function of temperature for $d=3$. Dashed and dotted lines are the underlying saddle energies for different sizes. $T_c=3.9573$ is the thermodynamic phase transition temperature.

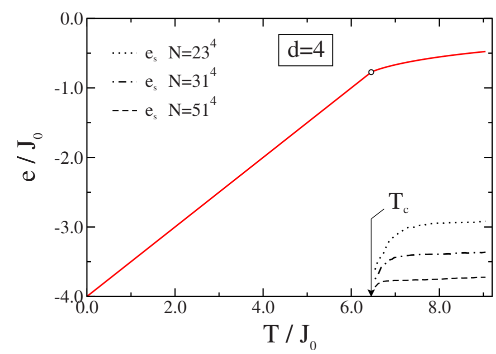

FIG. 2. (Color online) Energy as a function of temperature for $d=4$. Dashed and dotted lines are the underlying saddle energies for different sizes. $T_c=6.4537$ is the thermodynamic phase transition temperature.

III. THERMODYNAMICS

The thermodynamics can be exactly solved [17] and, in the canonical ensemble, the free energy density f turns out to be

$$-\beta f = -\frac{1}{2}(1+\ln 4K) + 2Kz - \frac{1}{2}g(z), \tag{6}$$

where $K=\beta J_0/2$ ($\beta=1/k_BT$, $k_B=1$ in the following) and

$$g(z) = \frac{1}{(2\pi)^d}\int_0^{2\pi} d\omega_1 \cdots d\omega_d \ln\Big(z - \sum_{i=1}^{d}\cos\omega_i\Big). \tag{7}$$

The variable z, as a function of β, $z(\beta)$, is the solution of the saddle point equation

$$4K = \frac{1}{(2\pi)^d}\int_0^{2\pi} d\omega_1 \cdots d\omega_d \frac{1}{z - \sum_{i=1}^{d}\cos\omega_i}, \tag{8}$$

or, in a more compact form,

$$4K = \int_0^{\infty} ds\, e^{-zs}[I_0(s)]^d, \tag{9}$$

with $I_0(s)=\int(d\omega/2\pi)\exp(s\cos\omega)$ the modified Bessel function of zeroth order.

A continuous phase transition takes place for $d\geq 3$. The energy density

$$e(\beta) = \begin{cases} \dfrac{1}{2\beta} - J_0 z(\beta) & \text{for } \beta<\beta_c, \\ \dfrac{1}{2\beta} - J_0 d & \text{for } \beta>\beta_c, \end{cases} \tag{10}$$

can be studied numerically and, as examples, it is shown in Figs. 1 and 2 (full lines) as a function of temperature T for $d=3$ and 4. The phase transitions are located at $T_c^{(3)}/J_0 \simeq 3.9573$ and $T_c^{(4)}/J_0 \simeq 6.4537$. respectively, corresponding to critical energy values $e_c^{(3)}/J_0 \simeq -1.0216$ and $e_c^{(4)}/J_0 \simeq -0.7728$ [16,17].

IV. TOPOLOGY

Topological quantities are related to stationary points of the potential energy. Indeed, the topology of the submanifold M_e can be investigated, using Morse theory, studying the critical values (corresponding to stationary points) of the potential energy function. For the spherical model critical points are, in fact, critical submanifolds (disjoint hyperspheres) [16]. There are $\hat{N}+1$ of such topological hyperspheres, whose dimension is given by the degeneracy d_i of the corresponding eigenvalue. Using the r_i variables—see Eq. (5)—the kth hypersphere is defined by $r_k=\sqrt{N}$, and $r_i=0$ for $i\neq k$. The energy of this critical manifold is $e_s^{(k)}=-J_0\hat{\lambda}_k/2$.

Risau-Gusman *et al.* [16] have shown that there is a continuum of topological transitions; however, abrupt (or strong) topological changes (supposed to be related to phase transitions [3,5]) are located at integer values of e/J_0, specifically, at odd values of e/J_0 for odd d, even values of $e/2J_0$ for odd $d/2$, and odd values of $e/2J_0$ for even $d/2$. These values do not correspond to the phase transition energies e_c/J_0. No strong topological discontinuity seems to be associated with the phase transition.

We suggest that a topology–phase-transition relationship could be established for this model, even though in a weaker sense, by looking at the underlying saddles.

V. UNDERLYING SADDLES

Underlying saddles are defined as the closest (with respect to the Euclidean distance in the configuration space) saddles to instantaneous configurations. We can then associate with any given configuration $\{x_i\}$ ($i=1,\ldots,N$)—corresponding to the set of values $\{r_i\}$, $i=0,\ldots,\hat{N}$; see Eq. (5)—the closest saddle (the critical hypersphere, in fact) $\{r_i^{(s)}\}$ ($i=0,\ldots,\hat{N}$) through the map

$$\mathcal{M}:\{x_i\} \rightarrow \{r_i^{(s)}\}, \tag{11}$$

with

$$r_k^{(s)} = \sqrt{N},$$

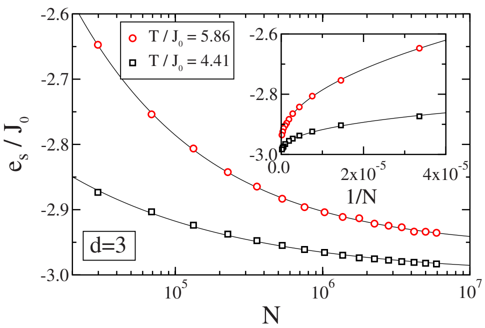

FIG. 3. (Color online) Saddle energy e_s as a function of system size for $d=3$ at two given temperatures. Inset: the same quantity versus the inverse size.

$$r_i^{(s)} = 0, \quad i \neq k, \quad \text{where} \quad r_k = \max_i r_i. \tag{12}$$

This follows immediately from the saddle point structure in configuration space (see previous section) and considering the minimum of $d^2=\Sigma_i(r_i-r_i^s)^2$ over the different saddles (we note that the distance d in r space corresponds to the minimum distance in configuration space between the given point $\{x_i\}$ and the points belonging to the considered critical hypersphere surface).

Writing the partition function in terms of r_i variables and considering Eq. (8)—which defines $z(\beta)$—the average saddle energy can be written as

$$e_s(\beta) = \int_0^\infty \prod_{i=0}^{\hat{N}} [dr_i P(r_i)] e_s^{(k)}, \tag{13}$$

where k is given by $r_k=\max_i r_i$ and

$$P(r_i) = \frac{2\alpha_i^{d_i/2}}{\Gamma(d_i/2)} r_i^{d_i-1} e^{-\alpha_i r_i^2} \tag{14}$$

with $\alpha_i=2K(z-\hat{\lambda}_i/2)$ and $\Gamma(x)=\int_0^\infty dt\, t^{x-1}e^{-t}$ is the Euler Gamma function. The quantity $e_s^{(k)}=-J_0\hat{\lambda}_k/2$ is the energy of the closest saddle to the sampled equilibrium configurations.

In Figs. 1 and 2 (dashed and dotted lines) the mean saddle energy as a function of temperature is shown for $d=3$ and 4. Different system sizes were used in the numerical calculation of e_s through Eq. (13). For all N the e_s curves approach the value $-J_0 d$ at the phase transition temperature T_c, $e_s(T_c)=-J_0 d$. In other words, when the system approaches the phase transition point, the underlying explored saddles approach the absolute minimum. It is worth noting that finite-size effects are relevant in determining the T dependence of the saddle energy e_s. Indeed, looking at the size dependence of e_s at fixed temperature (Figs. 3 and 4 for two given temperatures), a very slow approach to an asymptotic value is observed.

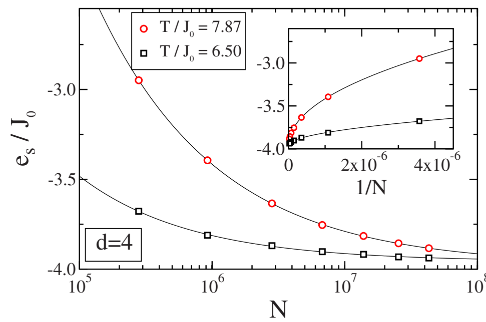

FIG. 4. (Color online) Saddle energy e_s as a function of system size for $d=4$ at two given temperatures. Inset: the same quantity versus the inverse size.

VI. CONCLUSIONS

Investigating the thermodynamics and topology of the d-dimensional spherical model, we have shown that underlying saddles play a central role in driving the phase transition. The map in the configuration space from instantaneous configurations to closest saddles relates the phase transition energy e_c to a critical topological value. In particular, the saddle energy goes to the minimum value at the phase transition point. The thermodynamic phase transition seems then to be related to the trivial critical topological value, i.e., the boundary energy $-J_0 d$: below T_c (and correspondingly below e_c) the system is always close to the minimum critical point (of energy $-J_0 d$), while above T_c (and e_c) the closest critical points are saddle points of growing energy. Even though, strictly speaking, for this model the (unconstrained) potential energy function cannot be considered a good Morse function—due to the constraint in Eq. (1)—and thus the observed discrepancy between topological and phase transition singularities should not be so surprising, it is quite remarkable that the "shortcut" represented by the weak topological hypothesis, which has been proven to work in different models [18,19], should also be satisfied by the d-dimensional spherical model investigated here. In other words, the hypothesized relationship between phase transitions and topological changes seems to be achieved by looking at the closest saddles in configuration space: the relevant topological information is stored in the saddles close to which the system is moving during the exploration of the whole configuration space. Whether the present findings are more general and have a deeper theoretical meaning remains a matter of future research.

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