Topological properties of the mean-field ϕ^4 model

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We study the thermodynamics and the properties of the stationary points (saddles and minima) of the potential energy for a ϕ^4 mean-field model. We compare the critical energy v_c [i.e., the potential energy $v(T)$ evaluated at the phase transition temperature T_c] with the energy v_θ at which the saddle energy distribution show a discontinuity in its derivative. We find that, in this model, $v_c \gg v_\theta$, at variance to what has been found in different mean-field and short ranged systems, where the thermodynamic phase transitions take place at $v_c = v_\theta$ [Casetti, Pettini and Cohen, Phys. Rep. **337**, 237 (2000)]. By direct calculation of the energy $v_s(T)$ of the "inherent saddles," i.e., the saddles visited by the equilibrated system at temperature T, we find that $v_s(T_c) \sim v_\theta$. Thus, we argue that the thermodynamic phase transition is related to a change in the properties of the inherent saddles rather than to a change of the topology of the potential energy surface at $T = T_c$. Finally, we discuss the approximation involved in our analysis and the generality of our method.

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I. INTRODUCTION

The investigation of the topological properties of the potential energy surface (PES) of liquids and disordered system [1] has been strongly revitalized in recent years [2–8]. These studies have been particularly focused on the connection between the slow dynamics of supercooled liquids and the properties of the stationary points of the potential energy function $V(q)$, q_i $(i = 1, \ldots, N)$ being the set of N generic configurational variables.

In the first approaches on studying the slow dynamics of supercooled liquids and glasses the objects of the investigations were the properties—energy location (v_m), curvature (ω_m), etc.—of the minima of the PES that are "visited" by the system during its evolution at a given thermodynamic state. Assigning to each minimum its basin of attraction, one obtains a partition of the configurational phase space: to each instantaneous configuration q, whose instantaneous potential energy is $v = V(q)/N$, one associates an "inherent" configuration q_m, whose potential energy is $v_m = V(q_m)/N$. This allows one to define a configurational entropy of the minima and a free energy for the supercooled and for the out-of-equilibrium glassy regime [9]. These properties of the minima of the PES were then connected to several features of supercooled liquids and glasses. Among them, we mention the *fragility* of the glass former [6,10,11], the diffusion processes in supercooled liquids [7,12–14], and the effective fluctuation-dissipation temperature [16] in the out-of-equilibrium glassy phase [15].

More recently this minima-based approach has been extended to consider also the other stationary points of the PES, namely, the saddle points. Using the saddle-based approach, it has been shown in Lennard-Jones-like liquids [17,18] and in p-spin mean-field systems [19] that the "order of the inherent saddles" (i.e., the number of negative eigenvalues of the Hessian matrix evaluated at the saddle points visited during the equilibrium dynamics at temperature T) extrapolates to zero when T reaches the dynamic transition temperature T_{MCT} (or mode-coupling temperature [22]). While the definition of "basin of attraction of a saddle" and the operative way to associate a saddle point with the instantaneous configuration of the system—i.e., the way to associate a saddle q_s [with energy $v_s = V(q_s)/N$] with each instantaneous configuration q (with energy v)—have been the subject of debate [23–25], the previous result has been shown to be robust and the method has been applied to other model systems [25–28]. In the following we will call a "map" the function that associates the thermal average of $v_s = V(q_s)/N$ with its parent $v = V(q)/N$, i.e., for each T, if $v(T)$ is the average potential energy and $v_s(T)$ the average potential energy of the saddle visited at temperature T, then the map is the function $\mathcal{M}$ such that $v_s(T) = \mathcal{M}(v(T))$. Until now, two different operative definitions of the saddle to be associated with an instantaneous configuration (two different maps) have been used. (1) In the numerical simulations of simple models, such as Lennard-Jones systems, a partitioning of the configuration space in basins of attraction of saddles is obtained via an appropriate function $W(q)$ [usually $W(q) = |\nabla_q V(q)|^2$] that has a local minimum on each stationary point of $V(q)$, and the saddles are then obtained via a minimization of $W(q)$ starting from an equilibrium configuration obtained from a molecular dynamics simulation at temperature T [17,18]. (2) In the analytic computations applied to disordered mean-field spin models one looks at the saddles that are closest, with respect to the distance in the configuration space, to a reference configuration extracted from the Gibbs distribution at temperature T [19]. In one specific case, the only one where this test has been performed, the two definitions have been proven to give identical results [8]. However, there are—to our knowledge—at least two other possible definitions of "basin of attraction of a saddle" that have never been tested in numerical simulation [20,21], and the problem of the proper definition of the saddles' basin is still open.

The role of the stationary points of the PES (saddles and minima) has been also pointed out in a different context. Recent studies aiming to clarifying the microscopic origin of *thermodynamic* phase transitions suggest that the presence and order of such transitions are related to changes in the topology of the manifold of the PES sampled by the system when crossing the critical point. More specifically the topology change is signaled by a discontinuity in (one of) the derivatives of the Euler characteristic. This function, determined by counting the number and the order of the stationary points of the PES, is a genuine topological property of the constant potential energy submanifold, and, in particular, it does not depend on the statistical measure defined on it (i.e., on temperature).

Before proceeding it is worth observing that the Euler characteristic $\chi(v)$ (that is used in the topological studies of the phase transitions) and the complexity of minima and saddles (which is the basic quantity in the investigation of the role played by the stationary points of the PES in determining the slow dynamics in disordered systems) have similar definitions. With $\mathcal{N}_\nu(v)$ the number of stationary points q_s of order ν (minima for $\nu=0$ and saddles for $\nu \geqslant 1$) that have potential energy $V(q_s) \leqslant Nv$, we can define the energy distribution of the stationary points

$$\Omega(v) = \sum_\nu \mathcal{N}_\nu(v), \tag{1}$$

and the Euler characteristic

$$\chi(v) = \sum_\nu (-1)^\nu \mathcal{N}_\nu(v). \tag{2}$$

It is clear that these two definitions are similar, but not coincident. Specifically, as $\mathcal{N}_\nu(v)$ is usually exponentially large in the size of the system N, $\Omega(v)$ can be evaluated at the saddle point in ν, thus defining an order $\overline{\nu(v)}$ that dominates in Eq. (1), while this procedure may not apply to $\chi(v)$ where large cancellations can arise from the term $(-1)^\nu$. The complexity (or configurational entropy) $\sigma(v)$ is defined as the logarithm of the number of stationary points whose energy lies in $[v, v+\delta v]$:

$$\sigma(v) = \frac{1}{N}\log\left(\frac{d\Omega(v)}{dv}\delta v\right) \sim \frac{1}{N}\log\,\Omega(v) \tag{3}$$

where the last approximation is promptly obtained recalling that $\Omega(v) \sim \exp N\sigma(v)$ is exponentially large in N. This scaling is not always found for the Euler characteristic which, at variance with $\sigma(v)$, can scale with N in many different ways [29]. We will further discuss this point in the following.

Following the numerical results obtained in [29] on the ϕ^4 model with nearest neighbor interactions in two and three dimensions, a theorem that relates the topological properties of the PES to the thermodynamic phase transitions has been recently demonstrated by Franzosi and Pettini for systems with generic short range interactions [30]. Though the theorem strictly applies to non-mean-field systems, the mean-field models examined so far seem to indicate the existence of a topology-thermodynamics relation for mean-field systems as well. In the (mean-field) XY model the (second order) phase transition, which takes place at a temperature T_c when the system is visiting the PES level given by $v_c = v(T_c)$, is signaled by a discontinuity in the first derivative of the Euler characteristic $\chi(v)$ at $v=v_c$ [31]. In the k-trigonometric model there is a phase transition, which is second order for $k=2$ and first order for $k>2$. For all k values, the phase transition is seen in the topology via a discontinuity in the first derivative of $\chi(v)$ at v_c, and the curvature of $\chi(v)$ around v_c gives also information on the order of the transition [32]. A detailed review of the previous results can be found in [33].

To summarize the previous paragraph, it seems that the relation between topology and thermodynamics is a general properties, being demonstrated for short range systems and tested via explicit computation of $\chi(v)$ for mean field system. There is, however, a simple counterexample: the mean-field ϕ^4 model [34–36]. In Ref. [36] it was observed that, for large value of the coupling parameters (J in the following nomenclature), the phase transition (second order, ferromagnetic-like) takes place at a temperature T_c where the equilibrium potential energy value v_c is *larger than the energy of the higher energy stationary point*, i.e., where $\chi(v)=1$ due to the Morse theorem [37] and, therefore, no discontinuity of $\chi(v)$ can be present. At this stage of the discussion it is worth pointing out a feature that is common to all the mean-field cases (XY and k-trigonometric for any k) where the topology-thermodynamics relation holds. Indeed, in these cases the energy of the "inherent" saddle visited by the system at T_c [i.e., $v_s(T_c)$] coincides with the instantaneous potential energy $v(T_c)$. In other words, for these systems, v_c is a fixed point for the map $\mathcal{M}:\mathcal{M}(v_c)=v_c$. Thus, the observed discontinuity of the derivative of $\chi(v)$ at v_c cannot discriminate between the two possibilities: (i) is the discontinuity in the topological properties *at the instantaneous* potential energy that marks the phase transition, or (ii) is the discontinuity in the topological properties *at the inherent saddles* potential energy that marks the phase transition. The ϕ^4 model does not share this peculiarity with the other investigated mean-field models, and can be therefore used to solve the ambiguity. While the Franzosi-Pettini theorem for non-mean-field systems seems to favor the possibility (i), the ϕ^4 model indicates that (i) is not applicable in mean-field systems. It is the aim of this work to test whether the possibility (ii) holds.

In this paper we first study the thermodynamics of the (symmetric) ϕ^4 model for different value of the coupling parameter J (the only independent parameter of the model), in order to individuate the temperature (T_c) and potential energy (v_c) location of the second order ferromagnetic phase transition. We then calculate the complexity of the stationary points of $V(q)$, namely, $\sigma(v)$, and we show that—at all J values—the discontinuity of the derivative of $\sigma(v)$ is found at a value (v_θ) which is always below v_c. Finally, we calculate the energy v_s of the inherent saddles [and thus the map $v_s=\mathcal{M}(v)$] in two different ways [minimization of $W(q)$ and lowest Euclidean distance], and we find that—within the small discrepancy existing between the maps determined in the two ways—the values of $\mathcal{M}(v_c)$ is very close to v_θ. The latter result indicates that on looking at the discontinuities of (the derivative of) the stationary points complexity one actually find a signature of the phase transition, but this signature is seen at the potential energy level of the "inherent" saddles, not at the instantaneous potential energy value. In other words, similar to what happens for the slow dynamics of disordered systems, it seems that are inherent saddle properties that determine the phase transitions in mean-field systems.

The paper is organized as follows: in Sec. II we present the model and its thermodynamical behavior; in Sec. III we study the properties of the stationary points of the potential energy and calculate their complexity; in Sec. IV and V we study the properties of the inherent saddles. Finally, we draw the conclusions.

II. THE MODEL

The ϕ^4 mean-field model describes N soft spins ϕ_i with a mean-field ferromagnetic interaction. Its thermodynamics, as well as its Langevin and Newton dynamics, have been studied in the literature; see, e.g., Ref. [35]. The model is defined by the (configurational) Hamiltonian

$$H = \sum_i h(\phi_i) - \frac{J}{2N}(\sum_i \phi_i)^2 = \sum_i h(\phi_i) - \frac{JNm^2}{2},$$

$$h(\phi) = -\frac{\phi^2}{2} + \frac{\phi^4}{4}, \tag{4}$$

where ϕ_i are real continuous variables and the magnetization m is defined as $m = N^{-1}\Sigma_i\, \phi_i$. Its thermodynamics can be exactly solved, as usual in mean-field models, in the thermodynamic limit. Defining

$$D\phi_i = d\phi_i \exp[-\beta h(\phi_i)], \tag{5}$$

the partition function is given by

$$\begin{aligned} Z_N(T) &= \int d\phi_i\, e^{-\beta H(\phi)} = \int D\phi_i \exp\left[\beta \frac{J}{2N}\left(\sum_i \phi_i\right)^2\right] \\ &= N \int dm\, e^{\beta JNm^2/2} \int D\phi_i \delta\left(Nm - \sum_i \phi_i\right) \\ &= N(2\pi)^{-1} \int dm\, d\hat{m}\, e^{\beta JNm^2/2 + iNm\hat{m}} \\ &\quad \times \int D\phi_i \exp\left(-i\hat{m}\sum_i \phi_i\right) \\ &= N(2\pi)^{-1} \int dm\, d\hat{m}\, e^{-\beta N f(m,\hat{m})} \end{aligned} \tag{6}$$

having defined

$$f(m,\hat{m}) = -\frac{Jm^2}{2} - iTm\hat{m} - T \log \int d\phi\, e^{-\beta[h(\phi) + i\hat{m}T\phi]}. \tag{7}$$

In the thermodynamic limit the free energy is obtained by evaluating the integral in Eq. (6) at the saddle point:

$$f(T) = -T \lim_{N\to\infty} N^{-1} \log Z_N(T) = \max_{m,\hat{m}} f(m,\hat{m}). \tag{8}$$

The saddle point equations can be written as

$$Jm = -iT\hat{m},$$

$$m = \int d\phi\, \mathcal{P}(\phi)\phi = \langle \phi \rangle_{\mathcal{H}}, \tag{9}$$

where we defined the single-particle Hamiltonian and the related Gibbs distribution

$$\mathcal{H}(\phi) = h(\phi) - Jm\phi,$$

$$\mathcal{Z} = \int d\phi\, e^{-\beta\mathcal{H}(\phi)},$$

$$\mathcal{P}(\phi) = \frac{e^{-\beta\mathcal{H}(\phi)}}{\mathcal{Z}}. \tag{10}$$

Having solved the self-consistency equation for the magnetization $m(T)$, $m = \langle\phi\rangle_{\mathcal{H}}$, the free energy is given by Eq. (8)

$$f(T) = \frac{Jm^2}{2} - T \log \mathcal{Z}. \tag{11}$$

As expected, the model undergoes a second order phase transition from a paramagnetic ($m = 0$) high-temperature phase to a ferromagnetic ($m \neq 0$) low-temperature phase. To find the critical temperature one has to expand the self-consistency equation for the magnetization in powers of m:

$$\begin{aligned} m &= \frac{\int d\phi\, \phi\, e^{-\beta h(\phi) + \beta Jm\phi}}{\int d\phi\, e^{-\beta h(\phi) + \beta Jm\phi}} \\ &= \beta Jm \frac{\int d\phi\, \phi^2\, e^{-\beta h(\phi)}}{\int d\phi\, e^{-\beta h(\phi)}} + o(m^3) \\ &= \mathcal{A}m + o(m^3). \end{aligned} \tag{12}$$

The transition temperature $T_c(J)$ is defined by the condition $\mathcal{A} = 1$, which gives

$$T_c = J \frac{\int d\phi\, \phi^2\, e^{-\beta_c h(\phi)}}{\int d\phi\, e^{-\beta_c h(\phi)}}. \tag{13}$$

The equilibrium potential energy is then given by

$$v(T) = \frac{d[\beta f(T)]}{d\beta} = \frac{Jm^2}{2} + \int d\phi\, \mathcal{P}(\phi)\, \mathcal{H}(\phi). \tag{14}$$

We will be interested in the average potential energy at the transition temperature, which—recalling that $m(T_c) = 0$—is given by

$$v_c = v(T_c) = \frac{\int d\phi\, h(\phi) e^{-\beta_c h(\phi)}}{\int d\phi\, e^{-\beta_c h(\phi)}}. \tag{15}$$

The behavior of the critical energy as a function of the coupling J is reported in Fig. 7 below.

III. TOPOLOGICAL PROPERTIES OF THE ENERGY SURFACE

In this section we will study the properties of the stationary points (saddles) of the potential energy surface of the system, defined by the Hamiltonian (4). We will now focus only on the *topological* properties of the saddles, while in Sec. IV we will study the properties of the saddles sampled by the system equilibrated at temperature T. Similar results, although obtained with a different procedure, have been discussed in Refs. [34,36].

A. Stationary points

The stationary points ϕ^s are defined by the condition $\nabla H(\phi^s)=0$, and their order ν is defined as the number of negative eigenvalues of the Hessian matrix $\mathrm{H}_{ij}(\phi^s) = (\partial^2 H/\partial\phi_i \partial\phi_j)|_{\phi^s}$. To determine the location of the stationary points we have to solve the system

$$\frac{\partial H}{\partial \phi_j} = -\phi_j + \phi_j^3 - Jm = 0 \quad \forall\, j. \tag{16}$$

We want to classify the stationary points of H according to their magnetization m and their energy $v=H(\phi^s)/N$. Thus, in Eq. (16) we will consider the magnetization m as a constant; this is exact in the $N\to\infty$ limit. Defining $\alpha=Jm$ and $\alpha_0 = 2/3\sqrt{3}$, the solutions of the equation $\phi^3-\phi=\alpha$ are given by

$$\phi_+(\alpha) = \frac{2}{\sqrt{3}} \cos\frac{\psi(\alpha)}{3},$$

$$\phi_0(\alpha) = -\frac{2}{\sqrt{3}} \cos\frac{\psi(\alpha)+\pi}{3},$$

$$\phi_-(\alpha) = -\frac{2}{\sqrt{3}} \cos\frac{\psi(\alpha)-\pi}{3},$$

$$\psi(\alpha) = \tan^{-1}(\alpha^{-1}\sqrt{\alpha_0^2-\alpha^2}), \tag{17}$$

and are such that $\phi_0(0)=0$, $\phi_\pm(0)=\pm 1$. For $\alpha=\pm\alpha_0$ we have $\phi_\mp=\phi_0$, while for $|\alpha|>\alpha_0$ two solutions become complex and only one solution can be accepted.

We will now restrict ourselves to the case $|\alpha|<\alpha_0$, and at the end we will discuss the case $|\alpha|\geqslant\alpha_0$. The stationary points of H are obtained by plugging a fraction $n_+=N_+/N$ of the ϕ_i in $\phi_i=\phi_+(\alpha)$, a fraction $n_0=N_0/N$ in $\phi_0(\alpha)$, and a fraction $n_-=N_-/N$ in $\phi_-(\alpha)$. Then, the energy v of the stationary point is given by Eq. (4):

$$v = \frac{H(\bar{\phi})}{N} = \sum_\xi n_\xi h(\phi_\xi(\alpha)) - \frac{\alpha^2}{2J} \tag{18}$$

where $\xi=(-,0,+)$. We can now determine the n_ξ by imposing the constraints

$$1 = \sum_\xi n_\xi,$$

$$\alpha = Jm = J\sum_\xi n_\xi\, \phi_\xi(\alpha),$$

$$v = \sum_\xi n_\xi\, h(\phi_\xi(\alpha)) - \frac{\alpha^2}{2J}. \tag{19}$$

The latter is a linear system that can be easily solved for any value of v, α; one must then impose the additional constraint $n_\xi \in [0,1]$ that restricts the allowed values of α and v. At given energy, we will have an interval $\alpha \in [\alpha_{min}(v), \alpha_{max}(v)]$ of allowed values of the magnetization. Recalling that a permutation of the ϕ_i does not change either the magnetization or the energy of the stationary point, the number of stationary points of magnetization α and energy v is simply given by

$$\frac{d\mathcal{N}}{dv}(\alpha,v) = \frac{N!}{N_+!\,N_0!\,N_-!} \sim \exp N\sigma(\alpha,v),$$

$$\sigma(\alpha,v) = \lim_{N\to\infty} N^{-1} \log\frac{dN}{dv}(\alpha,v) = -\sum_\xi n_\xi \log n_\xi. \tag{20}$$

To compute the order of the stationary point, we need the expression of the Hessian matrix. It is given by

$$\mathrm{H}_{ij} = (3\phi_i^2 - 1)\delta_{ij} - \frac{J}{N}. \tag{21}$$

In the thermodynamic limit it becomes diagonal,

$$\mathrm{H}_{ij} = (3\phi_i^2 - 1)\delta_{ij}. \tag{22}$$

One cannot *a priori* neglect the contribution of the off-diagonal terms to the eigenvalues of H, but one can prove [36] that their contribution changes the sign of at most one eigenvalue out of N. Neglecting the off-diagonal contributions, one can easily realize that the number of negative eigenvalues of H_{ij} is given by the number of $\phi_i=\phi_0(\alpha)$; then $\nu=Nn_0(\alpha,v)$. To summarize, we obtained the following results for $|\alpha|<\alpha_0$.

(i) The stationary points are classified according to their magnetization $m=\alpha/J$ and their potential energy v: from Eqs. (19) one can determine the fraction $n_\xi(\alpha,v)$ of $\phi_i=\phi_\xi(\alpha)$.

(ii) The number of stationary points of magnetization α and energy v is given by $\exp N\sigma(\alpha,v)$, where $\sigma(\alpha,v) = -\Sigma_\xi\, n_\xi(\alpha,v)\log n_\xi(\alpha,v)$.

(iii) The stationary points of magnetization α and energy v have order $\nu=Nn_0(\alpha,v)$.

We will now consider the case $\alpha=\alpha_0$ (the case $\alpha=-\alpha_0$ gives the same results from symmetry arguments). The equation $\phi^3-\phi=\alpha_0$ admits only two solutions, namely, $\phi_+=2/\sqrt{3}$ and $\phi_0=-1/\sqrt{3}$. Thus, in this case, we impose only the first two constraints:

$$1=\sum_\xi n_\xi = n_0+n_+,$$

$$\alpha_0 = J\sum_\xi n_\xi\phi_\xi = -J\frac{n_0}{\sqrt{3}}+J\frac{2n_+}{\sqrt{3}},$$

from which we get $n_0=\frac{2}{3}(1-1/3J)$ and $n_+=\frac{1}{3}(1+2/3J)$. Note that from the condition $n_0,n_+\in[0,1]$ these stationary points exist only for $J\geqslant 1/3$. Their energy is given by

$$v_0(J) = -\frac{1}{6}\left(1+\frac{5}{9J}\right). \tag{23}$$

These stationary points are characterized by an extensive number (n_0N) of zero eigenvalues of the Hessian matrix associated with $\phi_i=\phi_0$. The remaining eigenvalues are positive as they are associated with $\phi_i=\phi_+$.

Finally, we consider the case $\alpha>\alpha_0$. In this case, there is only one real and positive solution ϕ_+ of the equation $\phi^3-\phi=\alpha$; then $\phi_i=\phi_+$ for all i and from the self-consistency equation $\alpha=JN^{-1}\Sigma_i\ \phi_i=J\phi_+$ we get

$$\phi_+^3-\phi_+=J\phi_+ \tag{24}$$

so that $\phi_+=\sqrt{J+1}$. Finally, we have to check that $\alpha=J\sqrt{J+1}>\alpha_0$, and this happens only for $J>1/3$. Thus, these two points (the latter and the similar one with negative magnetization) exist only for $J>1/3$ and represent the absolute (magnetic) minima of the system. Their energy is given by $v_M=-(1+J)^2/4$.

B. Configurational entropy

The configurational entropy $\sigma(v)$ of the stationary points is defined in Eq. (1). It can be written as

$$\sigma(v) = N^{-1}\log\int_{\alpha_{min}(v)}^{\alpha_{max}(v)} d\alpha\, e^{N\sigma(\alpha,v)}$$
$$= \max_{\alpha\in[\alpha_{min}(v),\alpha_{max}(v)]}\sigma(\alpha,v). \tag{25}$$

We will neglect the contribution coming from the absolute minima (their number being nonextensive) and from the points with $\alpha=\alpha_0$ as they exist only for a particular value of v at which—as we will see—$\sigma(v)$ displays a singular behavior. Then, for any given energy v we can find $\overline{\alpha}(v)$ such that $\partial\sigma/\partial\alpha=0$ and $\sigma(v)=\sigma(\overline{\alpha}(v))$. Correspondingly, we can define the average saddle order $\overline{n}(v)=n_0(\overline{\alpha},v)$.

C. Euler characteristic

The Euler characteristic is defined in Eq. (2) and can be written as

$$\chi(v) = \int_{-\infty}^{v} du\int_{\alpha_m(u)}^{\alpha_M(u)} d\alpha\, e^{N[\sigma(\alpha,u)+i\pi n_0(\alpha,u)]}, \tag{26}$$

recalling that $\nu=Nn_0(\alpha,u)$ is the order of the stationary points of magnetization α and energy u. One can attempt to calculate the integral via the saddle point approximation: one has then to find the stationary points of the function

$$f(\alpha,u)=\sigma(\alpha,u)+i\pi n_0(\alpha,u) \tag{27}$$

with respect to the variables α and u. Moreover, α and u must be considered as complex variables as the function f has a nonvanishing imaginary part. However, in the model under discussion, at least at low v, the saddle point either does not exist or is not on a path going from α_{min} to α_{max} on which Re f is smaller than its value at the saddle point. Thus, we expect log $\chi(v)$ to be nonextensive at low v; in this case the saddle point approximation is not useful to evaluate $\chi(v)$ and one must take into account the strong cancellations between addends in Eq. (2). This point needs further investigation and we will not discuss it here. However, we stress that $\sigma(v)$ is probably very different from $\chi(v)$ at least at low energy.

D. Summary of the results

We will now summarize the topological behavior of the model at different values of J. All the results have been obtained by solving numerically the equation $\partial\sigma/\partial\alpha=0$ to calculate $\overline{\alpha}(v)$ and substituting it in the explicit expressions for all the other interesting quantities.

A first qualitative change in the topology is found at $J_1=1/3$, while a second is at $J_2=2$. We will now analyze in some detail the three regions of couplings: weak $(J<J_1)$, intermediate $(J_1<J<J_2)$, and strong $(J>J_2)$.

1. Weak coupling

In Fig. 1 we report the investigated quantities for $J=1/6<J_1$. In the top panel we report, as a function of the energy v, the minimum and maximum allowed values of α (dashed lines), together with the value $\overline{\alpha}(v)$ determined by the maximization of $\sigma(\alpha,v)$ (full line). Above $v=-1/4$, $\alpha_{min}=0$, while below $v=-1/4$, the paramagnetic $(\alpha=0)$ stationary points disappear and $\alpha_{min}>0$. In this $J<1/3$ region we have $\alpha_{max}<\alpha_0$ for any v. In the central panel we report the saddle order as a function of the energy. Above $v=-1/4$ there are no minima $(n_{min}>0)$ while below $v=-1/4$ minima and saddles coexist. The absolute minima are at $v_M\sim-0.34$, where $n_{max}\to 0$. Thus, there exist saddles of order $\nu>0$ arbitrarily close (in energy) to the absolute minima. In the bottom panel we report the configurational entropy as a function of v. From the top panel we see that there exists a value $v_\theta>-1/4$ (marked by the arrow) above which $\overline{\alpha}(v)=0$ while for $v<v_\theta$ we have $\overline{\alpha}(v)>0$. At the same energy the configurational entropy displays a singularity, but only in its second derivative; indeed, we have [recalling that, by definition of $\overline{\alpha}(v)$, $(\partial\sigma/\partial\alpha)(\overline{\alpha}(v),v)=0$]

$$\frac{d\sigma}{dv}=\frac{\partial\sigma}{\partial v}(\overline{\alpha}(v),v)+\frac{\partial\sigma}{\partial\alpha}(\overline{\alpha}(v),v)\frac{d\overline{\alpha}}{dv}=\frac{\partial\sigma}{\partial v}(\overline{\alpha}(v),v),$$

$$\frac{d^2\sigma}{dv^2}=\frac{\partial^2\sigma}{\partial^2 v}(\overline{\alpha}(v),v)+\frac{\partial^2\sigma}{\partial\alpha\,\partial v}(\overline{\alpha}(v),v)\frac{d\overline{\alpha}}{dv}, \tag{28}$$

so that the first derivative of σ is smooth while its second derivative is singular due to the singularity in $d\overline{\alpha}/dv$ at v_θ.

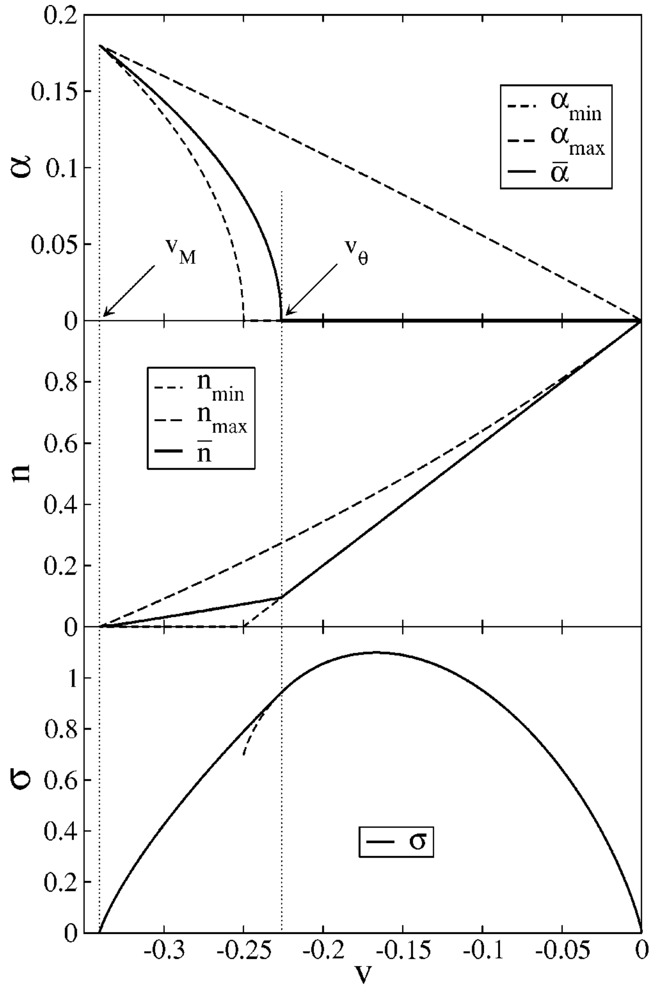

FIG. 1. Topological properties of the energy surface for $J=1/6$. Top panel: maximum and minimum allowed values for the magnetization of the saddles as a function of their energy (dashed lines) and the value $\overline{\alpha}(v)$ (full line) that corresponds to the maximum configurational entropy. Central panel: the maximum n_{max} and minimum n_{min} allowed values for the order of the saddles as a function of their energy (dashed lines) and the value $\overline{n}(v)$ (full line) that corresponds to the maximum configurational entropy. Bottom panel: total configurational entropy of the saddles as a function of v. For these values of J there is only one singularity v_θ below which $\overline{\alpha}\neq 0$.

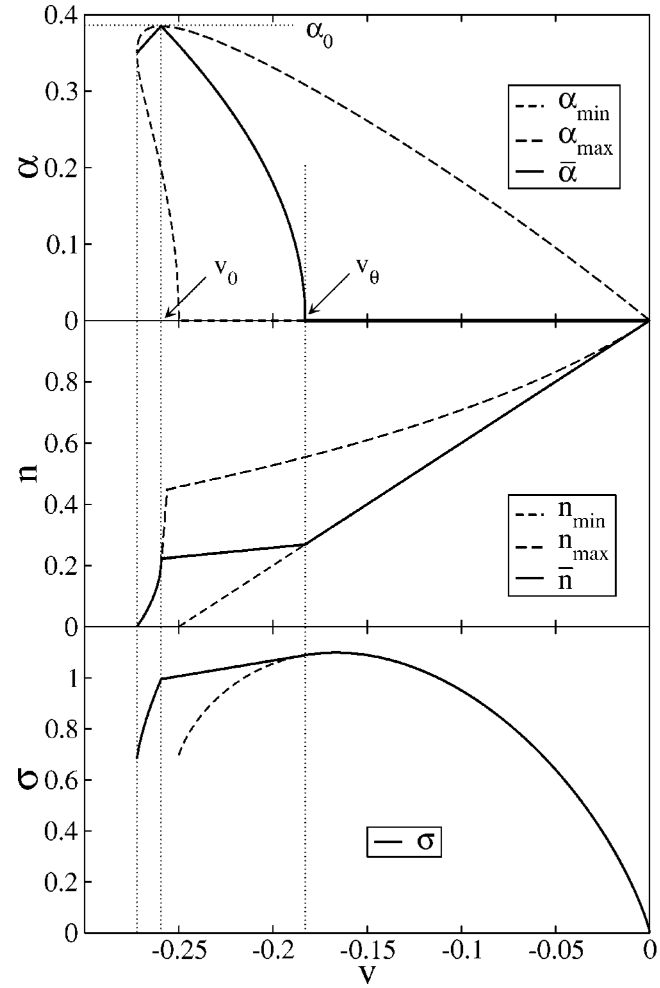

FIG. 2. Topological properties of the energy surface for $J=1$. The plots are the same as in Fig. 1. In this region a second singularity v_0 appears where $\overline{\alpha}=\alpha_0$. Below v_0 $\overline{\alpha}$ decreases again until v reaches its lowest possible value. In this region, the absolute minima are far below the minimum energy of the saddles and are not reported in the figure (see text).

The curve $\sigma(0,v)$ is reported as a dashed line. Note that even if for $v_M<v<-1/4$ there exist stationary points with fractional order $\nu/N=0$, we have $\overline{n}(v)>0$.

2. Intermediate coupling

In Fig. 2 the same quantities of Fig. 1 are reported for $J_1\leqslant J\leqslant J_2=2$ (namely, $J=1$). Again, we have a singularity at $v_\theta>-1/4$ where $\overline{\alpha}$ become different from 0. Moreover, in this region, the points with $\alpha=\alpha_0$ appear: as we can see from the upper panel, both α_{max} and $\overline{\alpha}$ move toward α_0 for $v\to v_0$. At $v=v_0$, we find $\overline{\alpha}=\alpha_0$; then for $v<v_0$ $\overline{\alpha}$ starts to decrease. The configurational entropy (lower panel) shows two singular points, the first at v_θ and the second at v_0. In the central panel the order of the saddles is reported. In this case, the minima are located at $v_M=-1$, well separated from the lowest order saddles. Then, in this case, a gap between the absolute minima and the lowest order saddles opens and $\overline{n}(v)$ goes to zero at a value $v>v_M$.

3. Strong coupling

At $J_2=2$ a third singularity $v_2<v_0<v_\theta$ appears, below which $\overline{\alpha}=0$ and again the paramagnetic saddles dominate. In Fig. 3 we report the results for $J=3>J_2$. We note that in this region we always have $\alpha_{min}=0$, while $\overline{\alpha}$ is zero for $v>v_\theta$, increases toward α_0 for $v_0<v<v_\theta$, and then decreases again and reaches zero at $v=v_2$, as previously discussed. The configurational entropy then follows the $\alpha=0$ curve apart from the interval $[v_2,v_\theta]$ in which it shows the additional singularity at v_0. In the inset of the lower panel we show the behavior of $\sigma(v)$ in the interval $[v_2,v_\theta]$. Again the absolute minima are at very low energy ($v_M=-4$) and are well separated from the lowest order saddles.

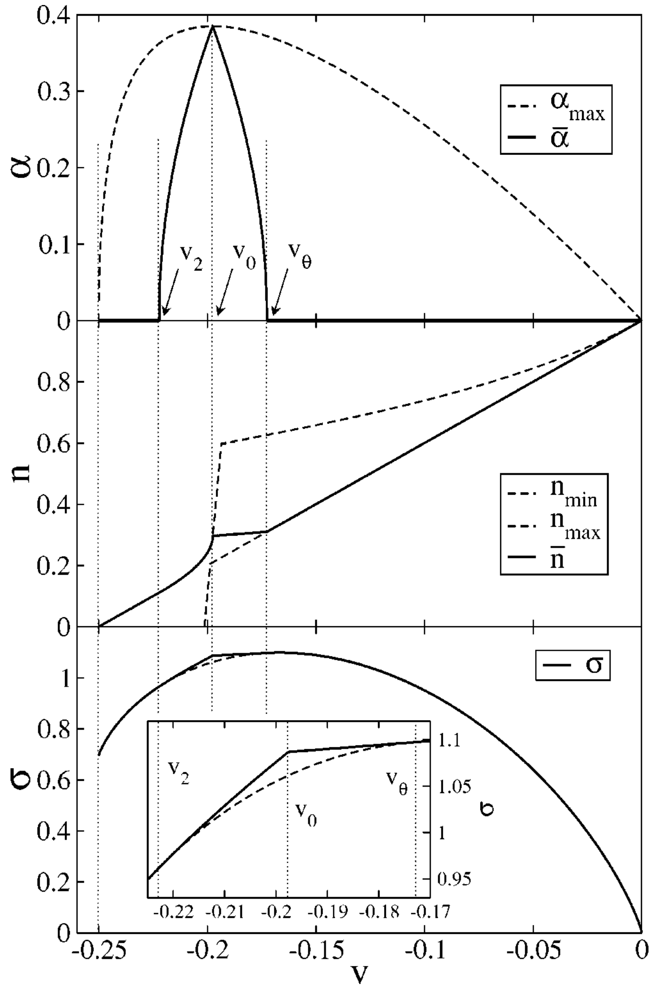

FIG. 3. Topological properties of the energy surface for $J=3$. The plots are the same as in Fig. 1. As in the previous figures there are two singularities of $\sigma(v)$ at v_θ and v_0. Moreover, in this region a third singularity v_2 appears below which again $\overline{\alpha}=0$. As in Fig. 2, the absolute minima are not reported in the figure. In the inset of the lower panel the region of the three singularities is magnified: one sees that $\sigma(v)$ is different from $\sigma(\alpha=0,v)$ only in the interval $v \in [v_2, v_\theta]$.

E. Discussion

As we discussed in the Introduction, it has been conjectured and verified in many different models [33] that topological singularities could be related to thermodynamic singularities (phase transitions) or dynamic singularities (glass transitions). We showed that the model has a very complex topological behavior. In particular, for $J<J_1$ there is only one singularity at $v=v_\theta$ below which the saddles are characterized by a "spontaneous magnetization;" for $J_1<J<J_2$ another singularity appears at $v=v_0<v_\theta$; the latter is due to the presence, at $v=v_0$, of points with magnetization $\alpha=\alpha_0$, characterized by a large number of zero eigenvalues of the Hessian matrix. For $J>J_2$, a third singular point v_2, below which the paramagnetic saddles again dominate, appears. However, for our discussion only v_θ will be relevant, as it represents the energy below which the saddles with $\alpha \neq 0$ become dominant, and hence could be expected to be related to the thermodynamical phase transition. If this is the case, one could expect the thermodynamical critical energy v_c to be close to v_θ.

In Fig. 7 below we report v_θ (full line) as a function of the coupling J together with the thermodynamical critical energy v_c (dot-dashed line). One immediately notices that v_c is far above v_θ, at variance to what is found in the previously investigated mean-field models [31,32] ; moreover, at high J one has $v_c>0$ while there are no stationary points of the Hamiltonian at positive energy, as already recognized in Ref. [36]. From this argument one concludes that, to relate the phase transition to changes in the topology of the PES one has to generalize in a suitable way the relation $v_c \sim v_\theta$ found in [31,32]. This will be the aim of the next section.

IV. INHERENT SADDLES

Recent works established that, in order to describe the equilibrium dynamics at a given temperature T, it is sufficient to know the properties of some of the stationary points, which have often been called "inherent saddles" [17–19,27]. To locate these particular stationary points, two main strategies have been adopted in the past: (1) partitioning the phase space in "basins of attraction" of stationary points via an appropriate function that has a local minimum on each stationary point; (2) defining in a proper way a "distance" in phase space and, given an equilibrium configuration, looking at the stationary point that has minimum distance from this configuration. It has been shown in [8] that, at least in a simple mean-field model, these two definitions give exactly the same result. In this section, we will discuss the properties of the inherent saddles using definition (2), which is more suitable for analiytical calculations, and later compare the results with the one obtained using definition (1).

To calculate the average energy and magnetization of the closest saddles to equilibrium configurations, we will make use of the method introduced in [19]. We compute the quantity

$$\Sigma(T;v_s,d) = \frac{1}{N}\int d\phi_i \, \frac{e^{-\beta H(\phi)}}{Z(T)} \log\Bigg(\int d\psi_i \; \delta(H(\psi) - Nv_s) \times \delta(\partial_i H(\psi)) \, |\det \mathrm{H}(\psi)| \; \delta(d^2 - d^2(\phi,\psi)) \Bigg)$$

where $\mathrm{H}_{ij}=\partial_i\partial_j H$ is the Hessian matrix and $d(\phi,\psi)$ is a distance function between the two configurations ϕ_i and ψ_i. The argument of the logarithm is the number of stationary points of energy v_s and distance d from the reference configuration ϕ (see Refs. [8,19] for a detailed discussion). Then the logarithm of this number (divided by N) is averaged over the equilibrium distribution at temperature T of the reference configuration. To find the closest saddles to equilibrium configurations—at given temperature T—we must find the minimum d such that $\Sigma(T;v_s,d) \geqslant 0$ (otherwise the number of saddles at distance d is zero). The condition $\Sigma(T;v_s,d) \geqslant 0$ will define a domain $\mathcal{D}_+$ in the (v_s,d) plane. We have then to find the minimum $d(T)$ of d in $\mathcal{D}_+$. Usually, this will correspont to a single value of v_s, which will be called $v_s(T)$ and represents the energy of the closest saddles. Note also that the point $(v_s(T), d(T))$ will be on the border of the domain $\mathcal{D}_+$ that is defined by the condition $\Sigma(T; v_s, d) \geq 0$; thus $\Sigma(T; v_s(T), d(T)) = 0$ [19,8].

In our model the distance function can be defined as

$$d^2(\varphi,\psi) = \frac{1}{N}\sum_i (\phi_i - \psi_i)^2. \tag{29}$$

The direct calculation of $\Sigma(T; v_s, d)$ is reported in the Appendix. There we show that the energy, distance, and magnetization of the closest saddles as a function of the temperature are given by the solution of the following equations:

$$\alpha = J \int d\phi\, \mathcal{P}(\phi)\, \tilde{\phi}(\phi,\alpha) = f(\alpha, T),$$

$$d^2(T) = \int d\phi\, \mathcal{P}(\phi)\, [\tilde{\phi}(\phi,\alpha) - \phi]^2,$$

$$v_s(T) = \frac{\alpha^2}{2J} + \int d\phi\, \mathcal{P}(\phi)\, \mathcal{H}(\tilde{\phi}(\phi,\alpha)), \tag{30}$$

where the function $\tilde{\phi}(\phi,\alpha)$ is equal to the $\phi_\xi(\alpha)$ such that $(\phi_\xi(\alpha) - \phi)^2$ is minimum, and $\mathcal{P}$ has been defined in Eq. (10). The first equation has to be interpreted as a self-consistency equation for α whose solution is the magnetization $\alpha_s(T)$ of the inherent saddles. Substituting $\alpha_s(T)$ in the second and third equations one gets the average distance $d(T)$ between equilibrium configurations and inherent saddles and the average energy $v_s(T)$ of the inherent saddles. Finally, substituting $\alpha_s(T)$ and $v_s(T)$ in the expression for the number of saddles and for their order derived in Sec. III we get the configurational entropy $\sigma(T)$ and the order $n_s(T)$ of the inherent saddles:

$$\sigma(T) = \Sigma(\alpha_s(T), v_s(T)),$$

$$n_s(T) = n_0(\alpha_s(T), v_s(T)). \tag{31}$$

Note that $\sigma(T)$ should not be confused with $\boldsymbol{\sigma}(T; v_s(T), d(T)) = 0$. In fact, the latter is the number of saddles of energy v_s subject to the additional constraint of having distance d from the equilibrium configurations, while the first is simply the number of saddles of energy v_s and magnetization α_s.

A. Properties of the inherent saddles

We will now discuss the properties of the inherent saddles in the weak and strong coupling regimes. We numerically solve the first of Eqs. (30) to get $\alpha_s(T)$, and from the other two we get all the quantities of interest.

1. Weak coupling

The behavior of the investigated quantities as a function of the temperature for $J = 1/6$ is reported in Fig. 4. In the top panel, the magnetization $\alpha_s(T) = Jm_s(T)$ of the closest saddles is reported together with the thermodynamic magnetization $Jm(T)$. We notice that $m_s(T) \sim m(T)$: thus, the system visits saddles that have a magnetization very similar to the equilibrium one. At low temperature, the system stays very close to the absolute minima (whose magnetization is reported as a dotted line) even if it reaches them only at $T = 0$. In the central panel, we report the energy $v_s(T)$ of the inherent saddles (dotted line) and the equilibrium energy $v(T)$ (full line). At $T = T_c$, both $v(T)$ and $v_s(T)$ show a singular behavior. We can observe that, in the present model, the saddle energy at T_c is smaller than the equilibrium energy, i.e., $v_s(T_c) = \mathcal{M}(v_c) < v_c$. This finding is at variance with the *XY* and *k*-trigonometric models where one finds $\mathcal{M}(v_c) = v_c$ [8]. We observe that the value of $v_s(T_c)$, for $J = 1/6$, turns out to be $v_s(T_c) = -0.212$, very close to $v_\theta = -0.226$. At low temperature $v_s(T)$ is very close to the energy of the absolute minima. Finally, in the lower panel, we report the saddle index $n_s(T)$. From the inset we see that, for $T \sim 0$, $n_s(T)$ has an Arrhenius behavior, $n_s(T) \sim \exp(-\Delta/T)$ [8].

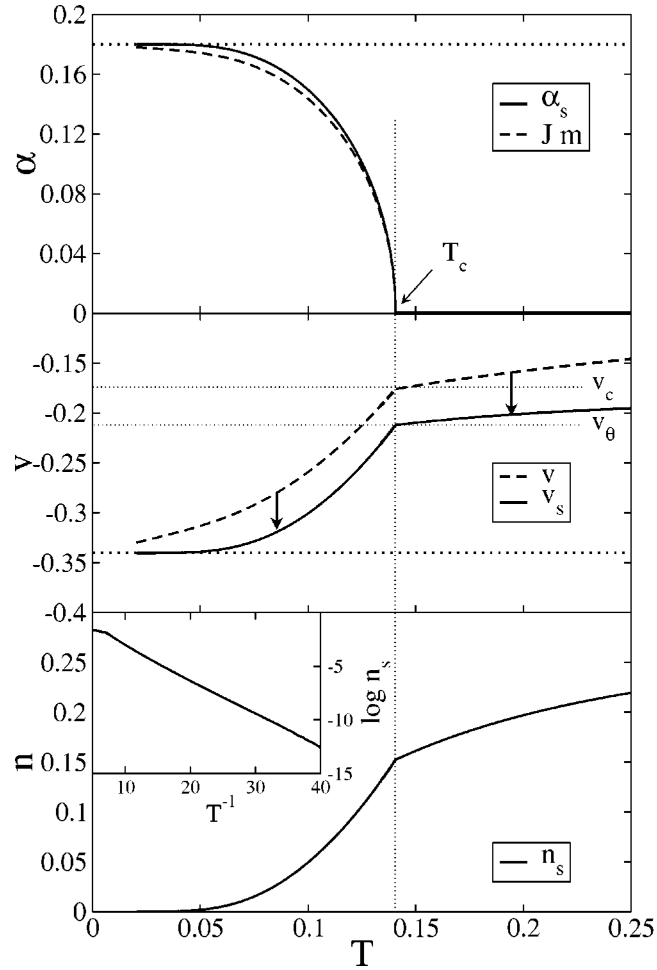

FIG. 4. Properties of the inherent saddles for $J = 1/6$ at different temperatures T. Top panel: magnetization $\alpha_s(T)$ of the closest saddles and magnetization $Jm(T)$ of the equilibrium configurations. Central panel: thermodynamical energy $v(T)$ and energy $v_s(T)$ of the closest saddles. The arrows graphically show the mapping $\mathcal{M}$ of the istantaneous energy into the inherent saddles energy. Bottom panel: saddle order $n_s(T)$. In the inset, $\log n_s$ is reported as a function of T^{-1} to enhance the low temperature Arrhenius behavior, $\log n_s = -\Delta/T$.

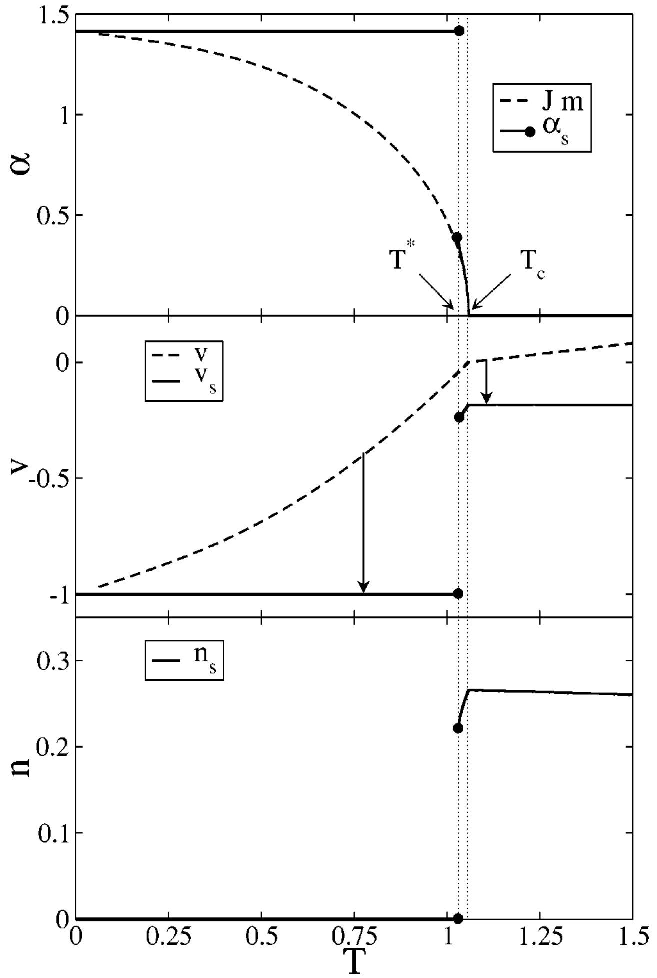

FIG. 5. Properties of the inherent saddles for $J=1$ at different temperatures T. The plots are the same as in Fig. 4. In the strong coupling regime the system jumps discontinuously in the minima at temperature T^* (marked by black dots in the figure).

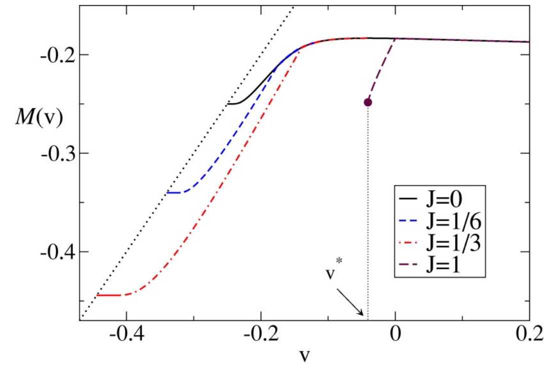

FIG. 6. The function $\mathcal{M}(v)$ that associates with the thermodynamic energy v the corresponding inherent saddle energy v_s for different values of J. The system follows the $J=0$ curve in the paramagnetic phase while below T_c the inherent saddles have lower energy with respect to that visited at $J=0$. At $T=0$ the system is in the minima and $v_s=\mathcal{M}(v)=v$ (dotted line). For $J>1/3$ the system jumps discontinuously into the minima at a certain energy $v^*=v(T^*)$ (full dot in the figure).

2. Intermediate coupling

In the intermediate and strong coupling regimes ($J>1/3$) the topology of the PES is very complicated, as we showed in the previous section (see Figs. 2 and 3). In particular, in this region the minima are separated from the lower energy saddles by a gap and two (or three) topological singularities appear. In Fig. 5 we report as an example the behavior of the magnetization, energy, and order of the inherent saddles as a function of the temperature for $J=1$. We see that as in the weak coupling regime the system samples nonmagnetized saddles above T_c while below T_c one has $\alpha_s(T)\neq 0$. However, at a given temperature T^* the system jumps discontinuously into the minima: below T^* the saddle order is exactly 0, the energy is $v_s(T)=v_M=-(1+J)^2/4$ and the magnetization is $\alpha_s=J\sqrt{1+J}$. On increasing J, T^* moves toward T_c. Note that there is no qualitative difference between the intermediate ($J<2$) and strong ($J>2$) coupling as the low energy saddles that are slightly below the gap are never visited by the system.

B. Mapping the instantaneous energy into the inherent saddles energy

As we discussed in the previous section, the equilibrated system at temperature T is close to saddles that have energy $v_s(T)<v(T)$, where $v(T)$ is the thermodynamical energy. We can construct the function $\mathcal{M}$ that maps the instantaneous energy v into the inherent saddles energy $v_s=\mathcal{M}(v)$ using the temperature as a parameter. The function $\mathcal{M}$ is reported in Fig. 6 as a function of v for selected J values. To check whether the energy of the inherent saddles at T_c is close to the singularity v_θ, we need to compute $v_s(T_c)=\mathcal{M}(v_c)$. We can obtain an explicit expression for $v_s(T_c)$ recalling that, for $T\geq T_c(J)$, we have $m(T)=0$, and $\mathcal{H}(\phi)=h(\phi)$. It is easy to see from Eq. (30) that $m=0$ implies $\alpha_s(T)=0$. Thus, in the paramagnetic phase the inherent saddles are always paramagnetic and their energy is given by the simple expression

$$v_s(T\geq T_c) = -\frac{1}{4}\left(1-\frac{\displaystyle\int_{-1/2}^{1/2} d\phi\, e^{-\beta h(\phi)}}{\displaystyle\int_{-\infty}^{\infty} d\phi\, e^{-\beta h(\phi)}}\right). \qquad (32)$$

The energy of the saddles sampled at T_c is simply given by the latter expression calculated in $T=T_c$. The energy of the inherent saddles at the critical temperature as a function of J is reported in Fig. 7 .

C. Discussion

As we showed in Sec. III, for the model investigated here, the energy at which the configurational entropy of the saddles shows a singularity (v_θ) is different from the energy at which the thermodynamical transition takes place (v_c) (see Fig. 7). Recent studies of the dynamics of glassy systems [17–19] demonstrated that the equilibrium properties at temperature T (and energy v) are related to the topological properties of the PES at energy $v_s=\mathcal{M}(v)$, i.e., the energy of the inherent saddles. If this is the case, one should expect the

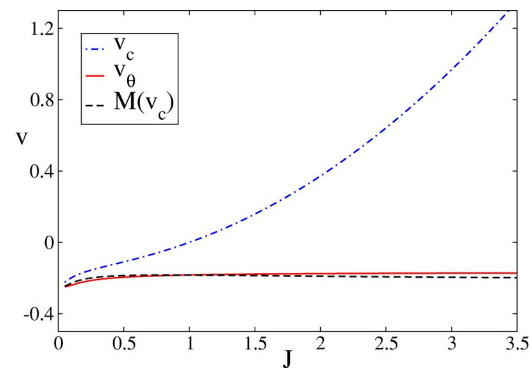

FIG. 7. The thermodynamical transition point $v_c = v(T_c)$ (dot-dashed line), the energy of the singularity of $\sigma(v)$, v_θ (full line), and the energy of the inherent saddles at T_c, $T_c = \mathcal{M}(v_c)$ (dashed line), as functions of the coupling J.

phase transition to happen when the energy of the inherent saddles (and not the thermodynamical energy) is close to the singularity v_θ of $\sigma(v)$. Indeed, as we can see from Fig. 7, the relation $\mathcal{M}(v_c) \sim v_\theta$ holds, even if not exactly. This result, the main finding of the present work, generalizes the relation $v_c \sim v_\theta$, discussed in Refs. [31–33,30] for cases where $\mathcal{M}(v_c) \sim v_c$, to the present case where $\mathcal{M}(v_c) \neq v_c$.

To better understand the origin of the small difference between $\mathcal{M}(v_c)$ and v_θ, in Fig. 8 we report (for $J=1/6$) the saddle order as a function of the saddle energy for (i) the saddles that dominate in the configurational entropy and (ii) the inherent saddles. As we clearly see from Fig. 8, the system is not always close to the saddles of order $\overline{n}$ that dominate in the configurational entropy (in the following, *dominant saddles*); indeed, below T_c the system start to sample saddles that are subdominant in the configurational entropy. However, one could expect the system to be always visiting the dominant saddles at energy $v_s(T)$, as the number of the dominant saddles is exponentially bigger than the number of all the other saddles. This discrepancy can be a consequence of an incorrect definition of the "basin of attraction" of a saddle, i.e., of an incorrect mapping between equilibrium

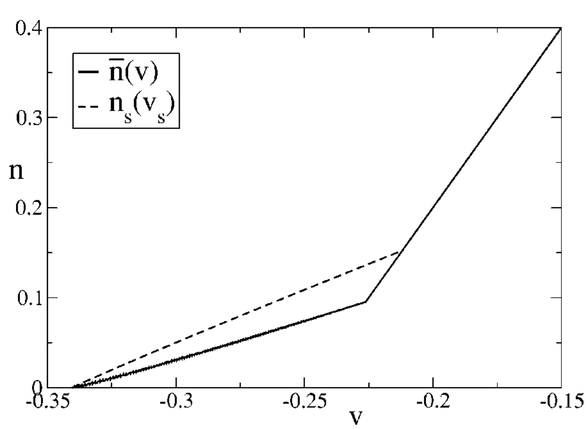

FIG. 8. Comparison between the order of the closest saddles (full line) and the order of the dominant ones (dashed line, see text) for $J=1/6$. $n_s(T)$ is reported as a function of $v_s(T)$ (see Fig. 4) parametrically in T while $\overline{n}(v)$ is the same as in Fig. 1.

configuration and inherent saddles. In the next section, we will discuss a different definition of the basin of attraction.

Finally, we observe that the physical interpretation of the discontinuous jump into the absolute minima that occurs for $J > 1/3$ is possibly related to the dynamical behavior of the system; the clarification of this point requires then the investigation of the dynamics of the system below T_c. Unfortunately, in Ref. [35] the Langevin dynamics of the system was studied only above T_c; the comparison of our results with the dynamical behavior of the system requires the extension of the calculations in Ref. [35] to the ferromagnetic phase.

V. DEPENCE ON THE DEFINITION OF BASIN OF ATTRACTION OF A SADDLE

As discussed in the introduction of this paper and in Ref. [8], the notion of "inherent saddles" can a *priori* depend on the way one defines the relation between an equilibrium configuration and the corresponding stationary point. We can try to examine what happens if we consider the definition (1) for inherent saddles, defining a new map $v_s = \mathcal{M}^W(v)$, at least in the paramagnetic phase where the calculation is straightforward. In this phase $m=0$ and $\mathcal{H}(\phi) = h(\phi)$. Thus the spins behave as if they were noninteracting ($J=0$). Thus, for $T > T_c$,

$$W(\phi) = |\nabla H|^2 = \sum_i \left| \frac{\partial h}{\partial \phi} \right|^2 = \sum_i |\phi_i^3 - \phi_i|^2 = \sum_i \phi_i^2(\phi_i^2 - 1)^2. \tag{33}$$

The minimization of W can be performed independently for each degree of freedom; the initial configuration ϕ is mapped in a configuration ϕ^s such that

$$\phi_i^s = \begin{cases} 1 & \text{if } \phi_i \geq \dfrac{1}{\sqrt{3}}, \\ 0 & \text{if } \phi_i \in \left[-\dfrac{1}{\sqrt{3}}, \dfrac{1}{\sqrt{3}} \right], \\ -1 & \text{if } \phi_i \leq -\dfrac{1}{\sqrt{3}}. \end{cases} \tag{34}$$

Recalling that h(0)=0 and $h(\pm 1) = -1/4$, we get (for $T > T_c$)

$$v_s^W(T) = -\frac{1}{4}\left(1 - \frac{\int_{-1/\sqrt{3}}^{1/\sqrt{3}} d\phi\, e^{-\beta h(\phi)}}{\int_{-\infty}^{\infty} d\phi\, e^{-\beta h(\phi)}} \right), \tag{35}$$

which differs slightly from the expression obtained in the previous section [Eq. (32)]—where the definition (2) of inherent saddles were used—as the interval of integration is different. Thus, the energy of the saddles sampled at temperature T depends slightly, in this model, on the definition of closest saddles to an equilibrium configurations, i.e., on the way one defines the basins of attraction of the saddles. In Fig. 9 we report, in an expanded scale with respect to Fig. 7, $\mathcal{M}^W(v_c)$ together with $\mathcal{M}(T_c)$ and with the singularity (in an expanded scale with respect to Fig. 7) of the configurational

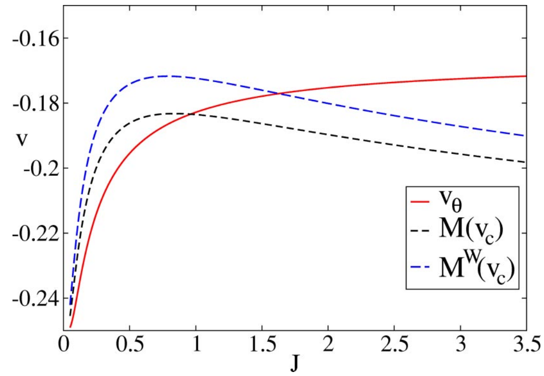

FIG. 9. The energy v_θ (full line), the energy $\mathcal{M}(v_c)$ of the closest saddles at temperature T_c (lower dashed line), and the energy $\mathcal{M}^W(v_c)$ of the saddles obtained by the minimization of W starting from an initial equilibrium configuration at temperature T_c (upper dashed line) as functions of J.

entropy v_θ. We see that the difference between $\mathcal{M}(v_c)$ and $\mathcal{M}^W(v_c)$ is of the same order as the difference between $\mathcal{M}(v_c)$ and v_θ. We conclude therefore that the relation $\mathcal{M}(v_c)\sim v_\theta$ holds within the approximations involved in the calculation of $\mathcal{M}(v_c)$.

VI. CONCLUSIONS

We characterized the properties of the stationary points of the potential energy surface of the ϕ^4 model and we compared them with the thermodynamical properties. We found that the singularity that is observed in the configurational entropy—not in the Euler characteristic—is located at an energy v_θ that is very close to the energy of the stationary points sampled by the system around the *thermodynamic* phase transition, $\mathcal{M}(v_c)$; we got then the relation $\mathcal{M}(v_c)\sim v_\theta$. In the previously investigated mean-field models [8,31,32] it was found that $\mathcal{M}(v_c)=v_c$ and that $v_\theta=v_c$; our result can be thought of as a generalization of the latter relation to the cases where the map $\mathcal{M}$ is not equal to the identity at T_c. However, some uncertainities in the determination of both v_θ and $\mathcal{M}(v_c)$ are present. Indeed, (i) v_θ is not a true topological singularity as it comes, in our analysis, from the configurational entropy which is not a topological invariant property of the energy surface; one should look at the Euler characteristic [33], which is, however, very difficult to determine in the present model due to strong cancellations between different saddle orders; and (ii) the exact value of $\mathcal{M}(v_c)$ has been shown to be slightly dependent on the way one associates with each configuration the corresponding inherent saddle; in particular, we showed that two different definitions of the inherent saddle give slightly different results, and that the difference is of the order of the difference between $\mathcal{M}(v_c)$ and v_θ.

The possible existence of a singularity in $\chi(v)$ at the critical energy v_c in the ϕ^4 mean-field model still remains an open problem that needs further investigation. Moreover, it seems that both the operative definitions of inherent saddle that have been used in the literature are unable to produce the expected relation $\mathcal{M}(v_c)=v_\theta$ exactly, even in such a simple model. Thus, from the present example one should conclude that the analysis of the thermodynamics in terms of the stationary points of the potential energy must be considered a useful but *approximate* tool, that has to be carefully used, evaluating case by case the domain of applicability of the method and the approximations that are necessarily involved.

ACKNOWLEDGMENTS

Recently, we became aware of work on the same subject by Garanin, Schilling, and Scala [38]. We thank them for sending us a copy of the work before its publication and for comments on our paper. We thank F. Sciortino and R. Franzosi for many useful comments and suggestions, and L. Casetti and M. Pettini for pointing out Ref. [36].

APPENDIX: CLOSEST SADDLES TO EQUILIBRIUM CONFIGURATIONS

In this section we will derive the result presented in Sec. IV. We have to compute the quantity

$$\sigma(T;v_s,d) = \frac{1}{N}\int d\phi_i \frac{e^{-\beta H(\phi)}}{Z(T)}\log\int d\psi_i\, \delta(H(\psi)-Nv_s) \times\delta(\partial_i H(\psi))\,|\det \mathrm{H}(\psi)|\,\delta(d^2-d^2(\phi,\psi)) \tag{A1}$$

where $d^2(\phi,\psi)=N^{-1}\Sigma_i(\phi_i-\psi_i)^2$. To do that, we need to prove a general relation. Suppose we want to calculate at the saddle point a quantity Q of the form

$$\begin{aligned} Q &= \frac{1}{N}\int d\phi_i \frac{e^{-\beta H(\phi)}}{Z(T)}\log A(\phi) \\ &= \lim_{n\to 0}\frac{1}{Nn}\left(\int d\phi_i \frac{e^{-\beta H(\phi)}}{Z(T)}A^n(\phi)-1\right) \\ &= \lim_{n\to 0}\frac{1}{Nn}\log\int d\phi_i \frac{e^{-\beta H(\phi)}}{Z(T)}A^n(\phi) \end{aligned} \tag{A2}$$

where we used the relations $\log x=\lim_{n\to 0}[(x^n-1)/n]$ and $\lim_{n\to 0}[f(n)-1]=\lim_{n\to 0}\log f(n)$ if $f(n)\to_{n\to 0}1$. In mean-field models, the energy is of the form $H(\phi)=\Sigma_i h(\phi_i)+Ne(m(\phi))$, where $Nm(\phi)=\Sigma_i m(\phi_i)$ [in our model, $m(\phi_i)=\phi_i$]. Then we have

$$\begin{aligned} Q &= \lim_{n\to 0}\frac{1}{Nn}\log\int dm\frac{e^{-\beta Ne(m)}}{Z(T)}\int D\phi_i\delta(m-m(\phi))A^n(\phi) \\ &= \lim_{n\to 0}\frac{1}{Nn}\log\int dm\, d\hat{m}\,\frac{e^{-\beta Ne(m)}}{Z(T)} \times\int D\phi_i \exp^{[i\hat{m}(Nm-\sum_i m(\phi_i))]}A^n(\phi) \\ &= \lim_{n\to 0}\frac{1}{Nn}\log\frac{1}{Z(T)}\int dm\, d\hat{m}\, e^{-\beta N[e(m)-Ts(n;m,i\hat{m})]} \end{aligned}$$

where we defined $D\phi_i=d\phi_i\exp[-\beta h(\phi_i)]$ and

$$s(n;m,i\hat{m}) = m\ i\hat{m} + \frac{1}{N}\log\int D\phi_i \exp\Big(-i\hat{m}\sum_i m(\phi_i)\Big)A^n(\phi).$$

Clearly $s(0;m,i\hat{m})$ is the entropic contribution to the free energy as a function of m, $\hat{m}$ that we obtain in the calculation of the partition function $Z(T)$, so that

$$f(T) = -\frac{1}{\beta N}\log Z(T) = \min_{m,\hat{m}}[e(m) - Ts(0;m,i\hat{m})]$$
$$= e(\mu) - Ts(0;\mu,\hat{\mu}) = f(0;\mu,\hat{\mu}), \qquad (A3)$$

where $(\mu(T),\hat{\mu}(T))$ is the (T-dependent) thermodynamic minimum of the free energy (note that at the saddle point $i\hat{m}=\hat{\mu}$). Then we have

$$Q = \lim_{n\to 0}\frac{1}{Nn}\log\int dm\ e^{-\beta N[f(n;m,i\hat{m})-f(0;\mu,\hat{\mu})]}. \qquad (A4)$$

We can now expand $m=\mu+n\mu^{(1)}+o(n^2)$, $i\hat{m}=\hat{\mu}+n\hat{\mu}^{(1)}+o(n^2)$, and

$$f(n;m,i\hat{m}) - f(0;\mu,\hat{\mu}) = \frac{\partial f}{\partial m}(0;\mu,\hat{\mu})n\mu^{(1)} + \frac{\partial f}{\partial i\hat{m}}(0;\mu,\hat{\mu})n\hat{\mu}^{(1)} + \frac{\partial f}{\partial n}(0;\mu,\hat{\mu})n + o(n^2) = \frac{\partial f}{\partial n}(0;\mu,\hat{\mu})n + o(n^2) \qquad (A5)$$

because by definition of $(\mu,\hat{\mu})$, we have $(\partial f/\partial m)(0;\mu,\hat{\mu})=0$, $(\partial f/\partial i\hat{m})(0;\mu,\hat{\mu})=0$. We get then the final result

$$Q = -\beta\frac{\partial f}{\partial n}(0;\mu,\hat{\mu}) = \frac{\partial s}{\partial n}(0;\mu,\hat{\mu}). \qquad (A6)$$

We have then to calculate (neglecting the term $\mu\hat{\mu}$ that vanishes on taking the derivative with respect to n)

$$s(n;\hat{\mu},v_s,d) = \frac{1}{N}\log\int D\phi_i \exp\Big(-\sum_i\hat{\mu}\phi_i\Big)\prod_{a=1}^{n}\int d\psi_i^a \times\delta(H(\psi^a)-Nv_s)\ \delta(\partial_i H(\psi^a)) \times|\det H(\psi^a)|\ \delta(d^2-d^2(\phi,\psi^a)) \qquad (A7)$$

where from the thermodynamic calculation (see Sec. II) $\hat{\mu}(T)=-\beta J\mu(T)$ and $\mu(T)$ is given by Eq. (9). We will now neglect the modulus of the determinant of the Hessian matrix replacing in the latter expression $|\det \mathrm{H}(\psi^a)|$ with $\det\mathrm{H}(\psi^a)$, in order to represent the determinant as an integral over fermionic variables. We will see later how to restore the correct sign in this term. Using a superfield representation [8] we get

$$s(n;\mu,v_s,d) = \frac{1}{N}\log\int D\phi_i \exp\Big(\beta J\mu\sum_i\phi_i\Big)\prod_{a=1}^{n}\int\frac{d\gamma_a}{2\pi} \times e^{N\gamma_a v_s}\int\mathcal{D}\Psi_i^a\exp\Big(\int d\bar{\theta}d\theta\,(1-\gamma_a\theta\bar{\theta}) \times H(\Psi^a)\Big)\delta\Big(Nd^2-\sum_i(\phi_i-\psi_i^a)^2\Big). \qquad (A8)$$

We will now (i) substitute the expression $H(\Psi^a)=\Sigma_i h(\Psi_i^a) - JNm(\Psi^a)^2/2$; (ii) insert some δ functions for $m_a=m(\Psi^a)$ and the corresponding integral representation with a multiplier $\hat{m}_a$; (iii) neglect all the product and sum signs related to the index a; (iv) use the integral representation for the δ function of d^2 with a multiplier λ_a. Then we get an expression that has to be maximized with respect to all the parameters to get the saddle point value of $s(n;\mu,v_s,d)$:

$$s(n;\mu,v_s,d) = \max_{\text{allpar}}\Bigg[\sum_a\gamma_a v_s - \sum_a\int d\bar{\theta}d\theta\Big((1-\gamma_a\theta\bar{\theta})\frac{Jm_a^2}{2} - m_a\hat{m}_a\Big) + \sum_a\lambda_a d^2 + \log\mathcal{S}(\mu,\hat{m}_a,\gamma_a,\lambda_a)\Bigg],$$

$$\mathcal{S}(\mu,\hat{m}_a,\gamma_a,\lambda_a) = \int d\phi\ \mathcal{D}\Psi^a\exp\Bigg[-\beta\mathcal{H}(\phi) + \sum_a\int d\bar{\theta}d\theta\,(1-\gamma_a\theta\bar{\theta})\,h(\Psi^a) - \sum_a\int d\bar{\theta}d\theta\,\hat{m}_a\Psi^a - \sum_a\lambda_a(\phi-\psi^a)^2\Bigg] \qquad (A9)$$

where $\mathcal{H}(\phi)=h(\phi)-J\mu\phi$ as in Eq. (10). As usual, we will assume that (i) there is symmetry between the replicas ($m_a=m$, etc.); (ii) all the fermionic components vanish at the saddle point. Then we get

$$s(n;\mu,v_s,d) = \max_{\text{allpar}}\Bigg\{n\Bigg[\gamma\Big(v_s+\frac{Jm_0^2}{2}\Big) - Jm_0m_3 + \hat{m}_0m_3 + \hat{m}_3m_0 + \lambda d^2\Bigg] + \log\mathcal{S}(\mu,\hat{m},\gamma,\lambda)\Bigg\},$$

$$\mathcal{S}(\mu,\hat{m},\gamma,\lambda) = \int d\phi e^{-\beta\mathcal{H}(\phi)}\Bigg[\int\mathcal{D}\Psi\ \exp\Big(\int d\bar{\theta}d\theta \times[(1-\gamma\theta\bar{\theta})h(\Psi)-\hat{m}\Psi]-\lambda(\phi-\psi)^2\Big)\Bigg]^n.$$

Now we have to take the derivative of s with respect to n at $n=0$. By direct computation

$$\sigma(\mu;v_s,d) = \max_{\text{allpar}}\frac{\partial s}{\partial n}(0;\mu,v_s,d) = \max_{\text{allpar}}\Bigg\{\Bigg[\gamma\left(v_s+\frac{Jm_0}{2}\right) - Jm_0m_3+\hat{m}_0m_3+\hat{m}_3m_0+\lambda d^2\Bigg] + \int d\phi\frac{e^{-\beta\mathcal{H}(\phi)}}{Z(T)}\log\int\mathcal{D}\Psi\,\exp\left(\int d\bar{\theta}d\theta \times[(1-\gamma\theta\bar{\theta})h(\Psi)-\hat{m}\Psi]-\lambda(\phi-\psi)^2\right)\Bigg\}. \tag{A10}$$

Some of the parameters can be easily eliminated computing the derivatives of σ; defining $\alpha=Jm_0$ one is left with the following expression:

$$\sigma(\mu;v_s,d) = \max_{\alpha,\gamma,\lambda}\Bigg[\gamma\left(v_s-\frac{\alpha^2}{2J}\right)+\lambda d^2 + \int d\phi\,\mathcal{P}(\phi)\,\log\sum_\xi e^{-\gamma\mathcal{H}(\phi_\xi(\alpha))-\lambda[\phi-\phi_\xi(\alpha)]^2}\Bigg] \tag{A11}$$

where $\mathcal{P}(\phi)$ is defined in Eq. (10), $\xi=(-,0,+)$ and the $\phi_\xi(\alpha)$ are defined in Eq. (17). Note that in the latter expression the term $\xi=0$ in the logarithm should have a minus sign: this is a consequence of the absence of the modulus of the determinant of the Hessian matrix that we neglected above. Taking the modulus into account corresponds to neglecting the minus sign of the term $\xi=0$. Performing the derivatives with respect to α, γ, and λ one obtains the following equations:

$$\alpha = J\int d\phi\,\mathcal{P}(\phi)\sum_\xi\mathcal{P}_\xi(\phi,\gamma,\lambda)\;\phi_\xi(\alpha)$$

$$d^2 = \int d\phi\,\mathcal{P}(\phi)\sum_\xi\mathcal{P}_\xi(\phi,\gamma,\lambda)\,[\phi-\phi_\xi(\alpha)]^2$$

$$v_s = \frac{\alpha^2}{2J}+\int d\phi\,\mathcal{P}(\phi)\sum_\xi\mathcal{P}_\xi(\phi,\gamma,\lambda)\;\mathcal{H}(\phi_\xi(\alpha)) \tag{A12}$$

where

$$\mathcal{P}_\xi(\phi,\gamma,\lambda) = \frac{e^{-\gamma\mathcal{H}(\phi_\xi(\alpha))-\lambda[\phi-\phi_\xi(\alpha)]^2}}{\sum_\xi e^{-\gamma\mathcal{H}(\phi_\xi(\alpha))-\lambda[\phi-\phi_\xi(\alpha)]^2}}. \tag{A13}$$

We want now to minimize d^2 with the condition $\sigma=0$. It is easy to show from Eq. (A12) that $(\partial d^2/\partial\lambda)\leqslant 0$. Then we expect that the minimum distance is obtained in the $\lambda\to\infty$ limit (see Ref. [8] for a detailed discussion of this point). It is easy to see that

$$\lim_{\lambda\to\infty}\mathcal{P}_\xi(\phi,\gamma,\lambda) = \chi_\xi^\alpha(\phi) \tag{A14}$$

where the function $\chi_\xi^\alpha(\phi)$ is equal to 1 if $\phi_\xi(\alpha)$ is the closest to ϕ and 0 otherwise. Thus, if we define $\tilde{\phi}(\phi,\alpha)$ as

$$\tilde{\phi}(\phi,\alpha) = \sum_\xi\chi_\xi(\phi)\phi_\xi(\alpha) \tag{A15}$$

(i.e., $\tilde{\phi}$ is the closest ϕ_ξ to ϕ), in the $\lambda\to\infty$ limit Eqs. (A12) become

$$\alpha = J\int d\phi\,\mathcal{P}(\phi)\;\tilde{\phi}(\phi,\alpha)$$

$$d^2 = \int d\phi\,\mathcal{P}(\phi)\,[\phi-\tilde{\phi}(\phi,\alpha)]^2$$

$$v_s = \frac{\alpha^2}{2J}+\int d\phi\,\mathcal{P}(\phi)\;\mathcal{H}(\tilde{\phi}(\phi,\alpha)). \tag{A16}$$

The first of these equations has to be interpreted as a self-consistency equation that gives the value of the magnetization of the closest saddles to the equilibrium configurations, $\alpha_s(T)$. The second and third equations give the average distance $d^2(T)$ and the average potential energy $v_s(T)$. Finally, observing that

$$\lim_{\lambda\to\infty}\log\sum_\xi e^{-\gamma\mathcal{H}(\phi_\xi(\alpha))-\lambda[\phi-\phi_\xi(\alpha)]^2} = -\gamma\mathcal{H}(\tilde{\phi}(\phi,\alpha))-\lambda[\phi-\tilde{\phi}(\phi,\alpha)]^2 \tag{A17}$$

substituting the latter expression in Eq. (A11), and using Eqs. (A16) one obtains

$$\lim_{\lambda\to\infty}\sigma = 0 \tag{A18}$$

consistently with our initial assumption.

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