Relationship between phase transitions and topological changes in one-dimensional models

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We address the question of the quantitative relationship between thermodynamic phase transitions and topological changes in the potential energy manifold analyzing two classes of one dimensional models, the Burkhardt solid-on-solid model and the Peyrard-Bishop model for DNA thermal denaturation, both in the confining and nonconfining version. These models, apparently, do not fit [M. Kastner, Phys. Rev. Lett. **93**, 150601 (2004)] in the general idea that the phase transition is signaled by a topological discontinuity. We show that in both models the phase transition energy v_c is actually noncoincident with, and always higher than, the energy v_θ at which a topological change appears. However, applying a procedure already successfully employed in other cases as the mean field ϕ^4 model, i.e., introducing a map $\mathcal{M}: v \to v_s$ from levels of the energy hypersurface V to the level of the stationary points "visited" at temperature T, we find that $\mathcal{M}(v_c) = v_\theta$. This result enhances the relevance of the underlying stationary points in determining the thermodynamics of a system, and extends the validity of the topological approach to the study of phase transition to the elusive one-dimensional systems considered here.

I. INTRODUCTION

Phase transitions are a very well understood subject in statistical mechanics. They have been characterized in many different ways in the last century and many observables related to the phase transition (e.g., critical exponents, correlation lengths, etc.) have been computed and measured with very high accuracy [1].

Recently, a characterization of phase transitions has been proposed by Pettini and co-workers [2–5]. These authors conjectured that, for classical systems defined by a continuous potential energy function $V(\{q_i\}_{i=1,\ldots,N})$, a thermodynamic phase transition, occurring at a temperature T_c, is the manifestation of a topological discontinuity, taking place at a specific value $v(T_c) = N^{-1}\langle V(q) \rangle$ (where $\langle \cdot \rangle$ is the statistical average at temperature T) of the potential energy function V, or, more precisely, taking place on the hypersurface $\Sigma_v = \{(q_1,\ldots,q_N) \in \mathbb{R}^N | V(q_1,\ldots,q_N) = Nv\}$, at $v = v(T_c)$. The most striking consequence of this hypothesis is that the signature of a phase transition is present in the topology of the configuration space independently on the statistical measure defined on it.

The changes in the topology are identified through the Morse theory [6]: topological changes in a manifold like Σ_v are related to the presence of stationary points of V (points for which $\nabla V = 0$) at energy v. However, the precise meaning of the correlation between topological changes and phase transitions in the general case is still a open question. On the one hand there is a theorem of Franzosi and Pettini [5], asserting that, for "smooth, finite-range and confining microscopic interaction potentials V with continuously varying coordinates, …, a topology change of the $\{\Sigma_v\}_{v \in \mathbb{R}}$ at some v_θ is a *necessary* condition for a phase transition to take place at the corresponding energy … value" [5]. On the other hand, there are different numerical studies of various models

[3,7–14] (almost all with potentials V *not* fulfilling the hypotheses of the theorem) for which a variety of results has been obtained, some are in agreement with the "*topological hypothesis*" of Pettini and co-workers, others seem to indicate its failure.

It is important to underline that the theorem in Ref. [5] establishes a *necessary* condition for a phase transition to take place. The problem to find *sufficiency* conditions is still an open problem, as pointed out also by the proponents of the hypothesis. This question has been addressed in two recent papers, in Ref. [11] a one-dimensional model, the Burkhardt model with nonconfining potential (see below) was investigated, finding that a topological change is present without a phase transition at finite temperature; in Ref. [14] the mean field spherical ferromagnet was considered, and it was found that the same topological changes happen either in the absence or in the presence of a magnetic field, while in the latter case no phase transition occurs (it is worth noting, however, that these two models do not fulfill the hypotheses of the theorem in Ref. [5]). Moreover, in the thermodynamic limit, it is likely that, for any finite interval of energy $I = [v_1, v_2]$, there is always a stationary point of $V(q)$ with energy $v \in I$; thus, in the thermodynamic limit a topological change occurs with probability one in any finite interval of energy. Most of these topological changes are—obviously—not related to phase transitions, and indeed it seems that a topological change must be *strong enough* to be related to a thermodynamic phase transition (see Ref. [7] for a detailed discussion of this point). An indication coming from the analysis of the models cited above is that the presence of a phase transition should be related to the presence of a *singularity* in the Euler characteristic at a given energy v_θ. Thus, basically, the idea of the "*topological*" approach is that the phase transitions are correlated to abrupt changes in topological quantities defined on the stationary points of V (as, for example, the Euler characteristic).

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Another open question is the equivalence between the energies at which phase transition (v_c) and change in the topology (v_θ) take place. The original conjecture of Pettini and co-workers asserts that the two energies "*correspond*" (let us call this the *strong topological hypothesis*). To our knowledge there is only one system within the hypotheses of the theorem, the two dimensional φ^4 model [3], for which the equivalence has been numerically established. In the other two systems with long range interactions, thus out of the theorem hypotheses (the mean field XY model [7] and the mean-field k-trigonometric model [8,9]), the equivalence has been analytically proved. There are, conversely, analytical results for a different model system (mean field φ^4 model [10]) for which the correspondence does not hold, the energy v_c at which phase transition takes place is higher than the energy v_θ of the topological singularity (we stress here that also in this case the hypotheses of the theorem in Ref. [5] are not fulfilled).

The latter discussion is of particular importance, not only in the context of phase transitions, but also in analogy with glassy systems. These systems are characterized—at the mean field level—by a dynamical transition taking place at a given temperature T_{MCT} (or equivalently at energy v_{MCT}) predicted by mode-coupling theory, and a (hypothesized) true phase transition at a lower temperature T_K (Kauzmann temperature) or energy v_K. From numerical simulations of Lennard-Jones-type systems, one observes that the dynamical transition is strictly related to the properties of the saddles visited by the system [15,16]. The concept of "visited saddles" is quantitatively worked out defining a pseudopotential $W=|\nabla V|^2$ and minimizing it during the dynamic evolution of the system, thus obtaining a map $\mathcal{M}_q:q \to q_s$ associating to each equilibrium configuration point $q=\{q_1,\ldots,q_N\}$ a minimum q_s of W. When averaged over the dynamic trajectory one obtains an energy map, $\mathcal{M}:v \to v_s$. Absolute minima of W [having $W(q_s)=0$] correspond to stationary points (saddles and minima) of V. We note that the presence of local minima of W, with $W(q_s) \neq 0$ but small (corresponding to inflection directions in V profile), does not affect the result [17], the order of visited saddles (number of negative eigenvalues of the Hessian matrix of V) extrapolates to zero at T_{MCT}, and the energy of saddles stays always below the instantaneous energy. Moreover the true thermodynamic transition is achieved when the number of visited stationary points of order zero (minima of V) grows less than exponentially with the system size (in the glassy terminology when the "*configurational entropy*" or "*complexity*" goes to zero). Solvable mean field spin-glass models (p spins), which manifest the same phenomenology of structural glasses, corroborate these findings in an analytical way [18]. Then, what emerges from glassy systems, is the great importance of the *underlying* stationary points in the description of the various transitions (dynamical and thermodynamical) taking place in these systems. It is worth noting, however, that the consistency of this picture beyond mean field is still a matter of debate [19], and that the definition of the map $\mathcal{M}$ is not unique also at the mean field level, different definitions giving similar but not quantitatively equal results [10].

One can argue, in line with the "*topological*" approach to

phase transitions, that also for nonglassy systems the concept of *underlying* stationary points continues to be useful. It is important to emphasize that, in the study of the glass transition, is the discontinuity of the average density number of underlying stationary points that marks the dynamical transition at T_{MCT}. Driven by this observation, we recently proposed that the map $\mathcal{M}:v \to v_s$ must be applied in order to spot the phase transition, i.e., if a topological discontinuity exists at energy v_θ, the phase transition is expected at an energy v_c such that $\mathcal{M}(v_c)=v_\theta$. This has been proved to work (at least approximately) in those cases (e.g., the mean field φ^4 model) where the original "*strong topological hypothesis*" (i.e., coincidence between v_c and v_θ) failed. It is worth pointing out that those cases where it has been proved that $v_c \equiv v_\theta$ do not constitute counterexamples for the application of the map $\mathcal{M}$, as in all these cases it turns out that v_c is a fixed point for the map, i.e., $\mathcal{M}(v_c)=v_c$. In conclusion, for all the cases investigated so far [7–10], it results that whenever a phase transition (including also "dynamic" transitions as the glass transition in LJ liquids [15,16] and p-spin systems [18]) is present at a certain energy v_c, this transition is signaled by a discontinuity in the topology, specifically in the Euler characteristic or in the complexity, at an energy v_θ such that $\mathcal{M}(v_c)=v_\theta$. At variance with the original (*strong*) topological hypothesis, where it was supposed that $v_c=v_\theta$, we will refer to the latter conjecture as the *weak topological hypothesis*. Note that the *weak topological hypothesis*, at variance with the *strong topological hypothesis*, depends on the statistical measure, as the map $\mathcal{M}:v \to v_s$ is defined through an *average* over the dynamical trajectory (or, equivalently, over the statistical measure). We will discuss this point in detail in the following.

Two recent papers [11,12] addressed the question concerning the relationship between phase transitions and topology in one-dimensional models. Kastner [11] studied two versions of a solid-on-solid model, one showing a phase transition at finite temperature and the other not; he found that both models exhibit the same topological change, thus concluded towards an "unattainability of a purely topological criterion for the existence of a phase transition" [11]. Grinza and Mossa [12] considered the Peyrard-Bishop model [20,21], which exhibits both a phase transition and a change in the topology, but in this case v_c and v_θ are not coincident [22]. These papers contributed to extend the analyzed cases for the understanding of necessary and sufficient conditions for the *topological hypothesis*. However, they seem to reach contradictory results, one supporting and the other falsifying the topological hypothesis, even if the investigated models share many similarities.

The aim of this work is to try to clarify this apparent inconsistency with regard to what has been discussed above. In particular, we reanalyze the model investigated by Kastner and by Grinza and Mossa. As a result of this study (i) analyzing the Peyrard-Bishop model (PB) [20,21] we numerically show that the two energies, although different $v_c \neq v_\theta$, satisfy the "*weak topological hypothesis*," i.e., $\mathcal{M}(v_c)=v_\theta$. We also investigate a slight modification of the PB model (allowing nonconfined motion of the variables), where we are able to study the same quantities in absence of a thermodynamic phase transition at finite temperature, again finding

results in agreement with the "*weak topological hypothesis*." (ii) Analyzing the Burkhardt model we introduce a further parameter defining the position of the pinning potential, that can be moved from the origin, i.e., fully confining potential, to infinity, fully nonconfining potential. We found that the phase transition actually exists for *all* the position of the pinning potential, and its critical temperature goes continuously to infinity as the pinning potential position goes to infinity. Moreover, we found that also the generalized Burkhardt model falls into the class of systems that satisfy the "*weak topological hypothesis*," i.e., $\mathcal{M}(v_c) = v_\theta$. As the position of the pinning potential is moved toward infinity, the energy $v_s(T)$ of the "*underlying saddles*" tends to reach the energy v_θ at higher temperature; when the nonconfining limit is reached, $v_s(T) \lesssim v_\theta$ for all T. The topological singularity is visited only for $T \to \infty$ and this is the reason why the phase transition is not observed, i.e., $T_c \to \infty$.

The present findings support the idea that also in the case of one-dimensional models, the relevant topological quantity related to a phase transition is obtained from underlying stationary points obtained from the map $\mathcal{M}$. As we already noted, the choice of the map $\mathcal{M}$ is not univocal, we have chosen the one obtained through W (with some *ad hoc* modifications), however different choices are possible (we mention here, for example, the map obtained using Euclidean distances in configuration space [10,18]). The robustness of this conclusion with respect to the possible different choices of the map $\mathcal{M}$ is still an open question which goes beyond the scope of this paper.

II. THE MODELS

The one-dimensional models we study are all defined by the Hamiltonian $\mathcal{H} = \sum_{i=1}^{N} p_i^2/2m + V(\{q\}_{i=1,...,N})$ (m is the mass of each particle), where V is the potential energy. We consider two different classes of models. The first one, introduced by Burkhardt [23] as a model for localization-delocalization transition of interfaces, is defined by the potential energy $V^{(1)}$,

$$V^{(1)}(\{q\}_{i=1,...,N}) = \sum_{i=1}^{N} K|q_{i+1} - q_i| + \sum_{i=1}^{N} V_p^{(1)}(q_i), \quad (1)$$

where K measures the strength of the force between neighboring pairs, $V_p^{(1)}(q)$ is the on-site pinning potential, and periodic boundary conditions are assumed $q_{N+1} \equiv q_1$. We choose for $V_p^{(1)}(q)$ the following form:

$$V_p^{(1)}(q) = \begin{cases} +\infty & \text{for } q \leq 0, \\ 0 & \text{for } 0 < q < L, \\ -U_0 & \text{for } L \leq q \leq L + R, \\ 0 & \text{for } q > L + R, \end{cases} \quad (2)$$

that generalizes the original form in Ref. [23] introducing a parameter L that gives the position of the pinning potential (a square well of depth U_0 and width R, see Fig. 1) from the edge of the system. The case with $L = 0$ coincides with the original Burkhardt confining model, while the nonconfining case is retrieved in the $L \to \infty$ limit.
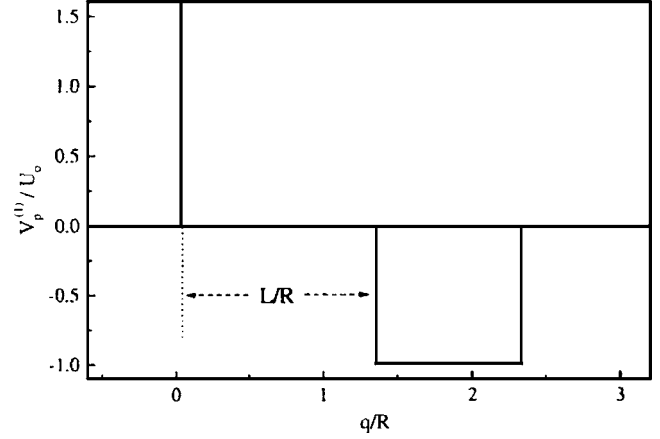

FIG. 1. Sketch of the on-site pinning potential $V_p^{(1)}(q)$ for a given choice of the control parameter L/R.

The models of the second class are defined by the potential energy $V^{(2)}$ and $V^{(3)}$ of the form

$$V^{(2,3)}(\{q\}_{i=1,...,N}) = \sum_{i=1}^{N} \frac{K}{2}(q_{i+1} - q_i)^2 + \sum_{i=1}^{N} V_p^{(2,3)}(q_i). \quad (3)$$

We consider two different versions of this model, one defined by the on-site Morse potential, introduced by Peyrard and Bishop as a simple model for DNA thermal denaturation [20,21] (PB model),

$$V_p^{(2)}(q) = U_0\{(e^{-q/R} - 1)^2 - 1\}; \quad (4)$$

the other is a symmetric version of the former (SPB model)

$$V_p^{(3)}(q) = U_0\{(e^{-|q|/R} - 1)^2 - 1\}, \quad (5)$$

a slight modification of PB model that allows for a nonconfined motion of the variables (see Fig. 2). We note that the introduction of the modulus in Eq. (5) does not introduce discontinuities up to the second derivative of the potential. The quantities U_0 and R determine respectively, the energy and the length scales of the on-site potential (in the following all quantities will be reported in U_0 and R units). We further
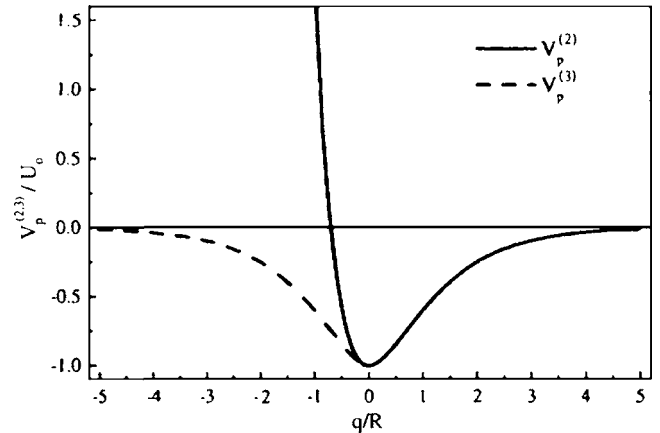

FIG. 2. Plots of the on-site pinning potentials $V_p^{(2)}(q)$ (full line) and $V_p^{(3)}(q)$ (dashed line).

choose $m=1$. In all three cases a parameter of the Hamiltonian is related to the strength of the interparticles interactions (K) and, for the case of $V^{(1)}$ a second parameter is the position of the pinning potential L.

Specifically, the relevant quantity defining the relative weight of the on-site with respect to interparticle potentials is the dimensionless ratio $\xi = KR/U_0$ or $\xi = KR^2/2U_0$ for the potential models (1) or (2) and (3), respectively, while the position of the pinning potential is given by $\zeta = L/R$ for the potential model (1).

The generalized Burkhardt model has been treated analytically, while the Peyrard-Bishop models are studied numerically. In the latter cases we performed isothermal molecular dynamics simulations using Nosé-Hoover thermostat at different temperatures for systems with $N=500$ degrees of freedom with periodic conditions $q_{N+1}=q_1$. We studied different values of the control parameter ξ, as an example the results are reported for $\xi=0.05$ and 0.5, all the other ξ values give results in qualitative agreement with the two reported examples.

III. BURKHARDT MODEL

A. Thermodynamics

The thermodynamics of the Burkhardt model has been known for many years [23] for both the $\zeta=0$ and $\zeta=\infty$ cases. The method of solution is briefly outlined below.

The determination of the thermodynamic of systems described by a potential function of the form

$$V(\{q\}_{i=1,\ldots,N}) = \sum_{i=1}^{N} K|q_{i+1} - q_i| + \sum_{i=1}^{N} V_p(q_i), \qquad (6)$$

i.e., similar to the case (1) [Eq. (1)], goes through the exploitation of the transfer matrix technique. Indeed, the configurational partition function $\mathcal{Z}$ is given by

$$\mathcal{Z}_N = \int dq_1 \cdots dq_N \, e^{-\beta V(\{q\}_{i=1,\ldots,N})}, \qquad (7)$$

that, defining the transfer "matrix"

$$\mathcal{T}(x,y) = e^{-\beta K|x-y|} e^{-\beta[V_p(x)+V_p(y)]/2}, \qquad (8)$$

can be written as

$$\mathcal{Z}_N = \int dq_1 \cdots dq_N \prod_{i=1}^{N} \mathcal{T}(q_i, q_{i+1}), \qquad (9)$$

recalling that $q_{N+1} \equiv q_1$. With this notation, the (configurational) free energy density

$$f = -\frac{1}{\beta N} \log(\mathcal{Z}_N) \qquad (10)$$

in the thermodynamic limit is promptly written as

$$f = -\frac{1}{\beta} \log(\max\{\bar{\lambda}\}), \qquad (11)$$

where $\bar{\lambda}$ is the set of eigenvalues of the transfer matrix, i.e., the eigenvalues of the integral equation

$$\int dy \, \mathcal{T}(x,y)\phi(y) = \lambda\phi(x). \qquad (12)$$

The latter equation, with the substitution

$$\psi(x) = e^{\beta V_p(x)/2}\phi(x), \qquad (13)$$

turns out to be

$$\int dy \, e^{-\beta K|x-y|} e^{-\beta V_p(y)}\psi(y) = \lambda\psi(x). \qquad (14)$$

The next step is performed by noticing that the operator $(-d^2/dx^2 + \beta^2 K^2)$ applied to $\exp(-\beta K|x-y|)$ produces a delta function,

$$\left(-\frac{d^2}{dx^2} + \beta^2 K^2\right) e^{-\beta K|x-y|} = 2\beta K \delta(x - y), \qquad (15)$$

thus by applying the previous operator to the integral equation (14), it can be transformed in a Schrödinger-type differential equation,

$$\left(-\frac{d^2}{dx^2} + \beta^2 K^2 - \frac{2\beta K}{\lambda} e^{-\beta V_p(x)}\right)\psi(x) = 0. \qquad (16)$$

This equation must be solved with the conditions that (i) the "eigenfunction" $\psi(x)$ was normalizable, and, (ii) the boundary condition [implicit in Eq. (14)] $\psi'(0)/\psi(0)=\beta K$ was fulfilled. In summary, the calculation of the thermodynamic system defined by the potential energy of the form in Eq. (1) is reduced to the solution of a Schrödinger-type differential equation and, in particular, to the finding of the largest eigenvalue of the original integral equation (14). In general, as the eigenvalues are continuous and smooth functions of the parameters (among which the temperature), no phase transitions are expected unless the two largest among them cross each other.

B. The $\zeta=0$ case

Let us now apply the procedure to the potential function in Eq. (1) for the case $\zeta=0$. We do not report the details of the calculation, as they are based on standard techniques for solving the Schrödinger equation in quantum mechanics [24]; in summary the "eigenvalues" λ are determined by the equation

$$z(\lambda) = \beta K \qquad (17)$$

with

$$z(\lambda) = \frac{f_1(P,Q)\sin(QR) - f_2(P,Q)\cos(QR)}{f_3(P,Q)\sin(QR) + f_4(P,Q)\cos(QR)}, \qquad (18)$$

having defined

$$f_1(P,Q) = Q^2,$$
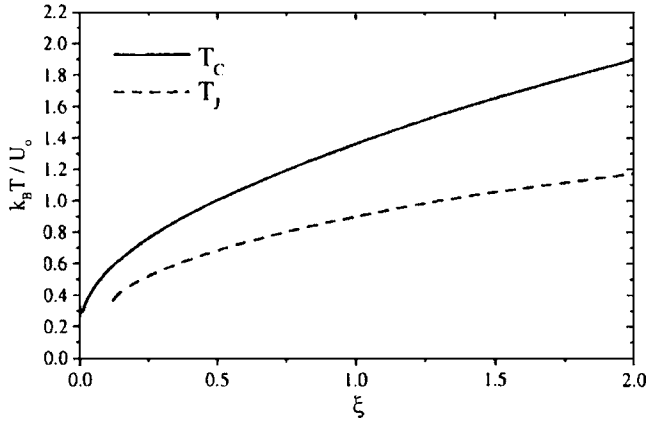
$$f_2(P,Q) = PQ,$$

$$f_3(P,Q) = P, \qquad (19)$$

FIG. 3. Full line, critical temperature (in reduced units $k_B T_c / U_0$) as a function of the control parameter ξ from Eq. (23) for the $\zeta = 0$ case. Dashed line, temperature T_J (in reduced units) at which the "underlying saddle" jumps from minimum to saddle as a function of ξ (see Sec. V B).

$$f_4(P,Q) = Q,$$

and

$$Q(\lambda) = \sqrt{\frac{2\beta K}{\lambda} e^{\beta U_0} - \beta^2 K^2},$$

$$P(\lambda) = \sqrt{\beta^2 K^2 - \frac{2\beta K}{\lambda}}. \qquad (20)$$

The only possibility for the function $z(\lambda)$ to be real [condition required for Eq. (17) to have a solution] is that P was real [if Q becomes imaginary, $z(\lambda)$ is still real], thus there is a solution to Eq. (17) only if P is real. Therefore, when P vanishes, the eigenvalues λ disappear (more specifically, the eigenvalues of the discrete spectrum disappear, and only those of the continuum spectrum remain), and the (configurational) free energy is discontinuous. For each temperature, the condition $P(\lambda) = 0$ is fulfilled for a "critical" λ, given by

$$\lambda_c = \frac{2}{\beta K}. \qquad (21)$$

Thus, the equation for the largest eigenvalue at the "critical" point is given by $z(\lambda_c) = \beta_c K$, or

$$\sqrt{e^{\beta_c U_0} - 1} \, \tan\left(\beta_c KR \sqrt{e^{\beta_c U_0} - 1}\right) = 1, \qquad (22)$$

which gives us the required equation for the critical (inverse) temperature β_c. This equation can be rearranged, introducing the control parameter $\xi = KR / U_0$, as

$$\xi = \frac{1}{\beta_c U_0} \frac{1}{\sqrt{e^{\beta_c U_0} - 1}} \arctan\left(\frac{1}{\sqrt{e^{\beta_c U_0} - 1}}\right). \qquad (23)$$

The plot of the critical temperature (in reduced units $k_B T / U_0$) as a function of ξ is reported as the full line in Fig. 3.

The phase transition is of the localization-delocalization type. The particles, kept together by the $K|x-y|$ term of the potential, for $T < T_c$ are pinned close to the square well, while, for $T > T_c$ are delocalized in the q axis.

A simple calculation leads to the value of the critical energy v_c [the equilibrium energy $v(T)$ at the transition point $v_c = v(T_c)$]. From Eq. (11), we have

$$v(T) = \frac{\partial(\beta f)}{\partial \beta} = -\frac{\lambda'(\beta)}{\lambda(\beta)}, \qquad (24)$$

where $\lambda(\beta)$ is the solution of Eq. (17). Close to the critical point, $\lambda(\beta) = 2/\beta K$, thus $\lambda'(\beta)/\lambda(\beta) = 1/\beta$ and

$$v_c = k_B T_c \qquad (25)$$

independently from the value of ξ.

C. The $\zeta \neq 0$ case

The calculation for the case of generic ζ values is quite similar to the previous one. Also in this case, the eigenvalues λ are determined by an equation like Eq. (17), $z(\lambda) = \beta K$, with $z(\lambda)$ again given by Eq. (18) and with the $f_n(P,Q)$ functions ($n = 1, …, 4$) given by

$$f_1(P,Q) = P[Q^2 \cosh(PR\zeta) - P^2 \sinh(PR\zeta)],$$

$$f_2(P,Q) = P^2 Q \exp(PR\zeta),$$

$$f_3(P,Q) = [P^2 \cosh(PR\zeta) - Q^2 \sinh(PR\zeta)], \qquad (26)$$

$$f_4(P,Q) = PQ \exp(PR\zeta).$$

Obviously, Eqs. (26) recover Eqs. (20) in the $\zeta \to 0$ limit. The same considerations on the reality of $P(\lambda)$ reported above apply to Eq. (26). Thus the condition $P(\lambda) = 0$ define the critical value of the eigenvalue, $\lambda_c = 2/\beta K$, and the equation for the critical temperature [$z(\lambda_c) = \beta_c K$] becomes

$$\sqrt{e^{\beta_c U_0} - 1} \, \sin(\beta_c KR \sqrt{e^{\beta_c U_0} - 1}) [\cos(\beta_c KR \sqrt{e^{\beta_c U_0} - 1})$$
$$- \beta_c KR\zeta \sqrt{e^{\beta_c U_0} - 1} \, \sin(\beta_c KR \sqrt{e^{\beta_c U_0} - 1})]^{-1} = 1. \qquad (27)$$

Similar to the $\zeta = 0$ case, this equation can be rearranged, introducing the control parameter ξ, as

$$\xi = \frac{1}{\beta_c U_0} \frac{1}{\sqrt{e^{\beta_c U_0} - 1}} \arctan\left(\frac{1}{\sqrt{e^{\beta_c U_0} - 1}} \frac{1}{1 + \beta_c U_0 \xi \zeta}\right). \qquad (28)$$

At variance with Eq. (23), this equation cannot be cast in the form $\xi = \xi(\beta_c)$, thus it must be solved numerically to plot the critical temperature as a function of the control parameter ξ. This plot is reported in Fig. 4 for different values of ζ.

As can be observed in Fig. 4, on increasing ζ, i.e., on displacing the position of the square well towards high value of the coordinate, the critical temperature, for a given ξ value, increases, expanding the amplitude of the "cold" (localized or pinned) phase. This can be better seen in Fig. 5, where the ζ dependence of the critical temperature is reported for some values of ξ. We conclude this section noticing that the phase transition actually exists for all the value of ζ, and in the limit of $\zeta \to \infty$, the critical temperature goes *without discontinuities* to infinity. Therefore, we are lead to conclude that the model investigated in Ref. [11] to demon-
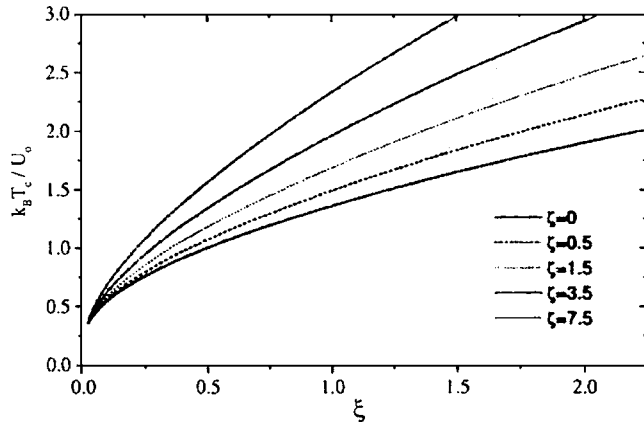
FIG. 4. Critical temperature (in reduced units $k_B T_c / U_0$) as a function of the control parameter ξ from Eq. (28) for the indicated ζ value, $\zeta = 0$ (full line), 0.5 (dashed line), 1.5 (dotted line), 3.5 (dashed-dotted line), and 7.5 (dashed-dotted-dotted line).

FIG. 6. Inverse temperature dependence (in reduced units βU_0) of the equilibrium potential energy for $\xi = 1$ and for the indicated ζ value, $\zeta = 0$ (full line), 0.5 (dashed line), 1.5 (dotted line), 3.5 (dashed-dotted line), and 7.5 (dashed-dotted-dotted line). The thick-dotted line represents the β dependence of the potential energy in the high temperature phase.

strate the unattainability of a purely topological criterion for the existence of a phase transition is a "borderline" model, in which the phase transition can be thought to be present at "T infinity" (even though the precise meaning of this statement is not well defined). Then, to the same topology [as we will see in the next section, the topology of the potential function in Eq. (2) does not depend on the value of ζ] always corresponds to a phase transition.

To discuss the question of the *coincidence* (or not) of the critical energy with the topological discontinuity, we need to calculate $v_c(\xi, \zeta)$. Following the same argument reported for the case $\zeta = 0$ we conclude that the critical potential energy depends on ξ and ζ only through $T_c, v_c = k_B T_c$. As an example, in Fig. 6 we report the caloric curve $v(T)$ as a function of the inverse temperature for different ζ values and for $\xi = 1$. For all the ζ values, on the low-β side the curves end at the points (β_c, v_c); these points are aligned along the $v_c(\beta_c)$ line (thick dotted line) given by $v_c(\beta_c) = 1 / \beta_c$.
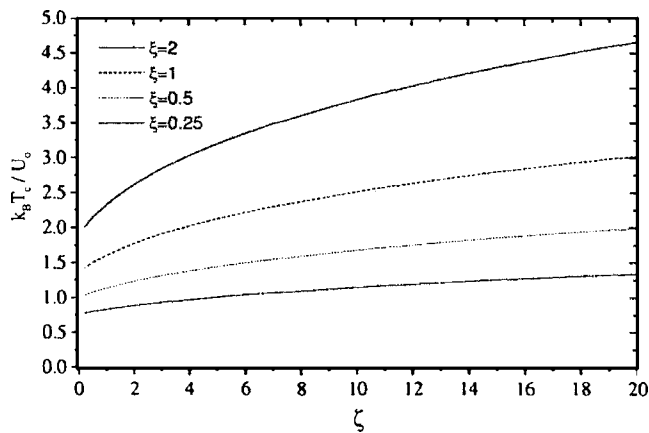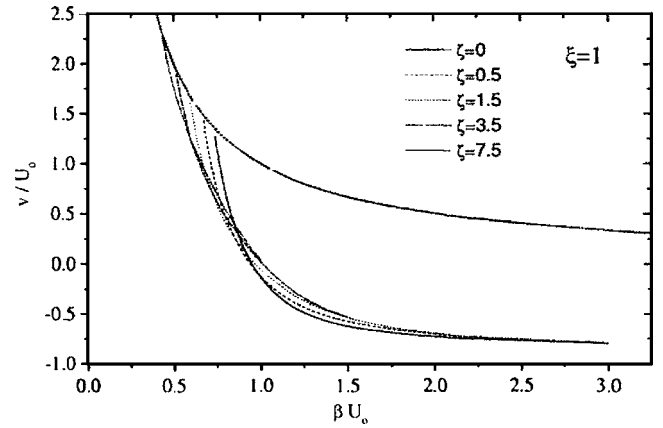
D. Topology

The analysis of the topological properties of the Burkhardt model is reported by Kastner in Ref. [11]. He analyzed only the two limiting cases of confining and non-confining models, corresponding in our notation to $\zeta = 0$ and $\zeta = \infty$, respectively. He found that a topology change is present in both cases, even if not really equal in "strength." The value of the potential energy at which the topological change appears is $v_\theta = 0$, irrespective of the considered model. One can easy generalize the above analysis to the general case with arbitrary ζ, and conclude that the topological change is always located at energy $v_\theta = 0$. It is worth noting that the energy at which topological change appears is lower than the thermodynamic transition energy, $v_c > v_\theta$ (see Fig. 6). We will further discuss this issue in Sec. VI, after having described the thermodynamics and topology of the PB and SPB models.

IV. PEYRARD-BISHOP MODEL

A. Thermodynamics

The thermodynamics of the Peyrad-Bishop model [defined in Eqs. (3) and (4)] can be studied using transfer matrix techniques, as the Burkhardt model described in the preceding section. However, in this case approximated methods must be considered in order to obtain a corresponding Schrödinger-type differential equation. In the region $\xi \gg 1$ and temperature window $U_0 \ll k_B T \ll \xi U_0$ the classical statistical mechanics problem is mapped to the quantum Morse oscillator problem [25,26]. Similarly to the case of Burkhardt potential, the presence of a second order phase transition for the Peyrad-Bishop model is signaled by the bounded-unbounded transition of the lower state in the corresponding quantum problem. In the above range of ξ and T, Peyrard and Bishop obtained an analytical expression for the transition temperature $k_B T_c / U_0 = 4 \sqrt{\xi}$ and transition energy $v_c / U_0 = k_B T_c / 2 U_0 = 2 \sqrt{\xi}$. For generic (ξ, T) values, only numerical

FIG. 5. Critical temperature (in reduced units $k_B T_c / U_0$) as a function of the control parameter ζ from Eq. (28) for the indicated ξ value, $\xi = 2$ (full line), 1 (dashed line), 0.5 (dotted line), 0.25 (dashed-dotted line).
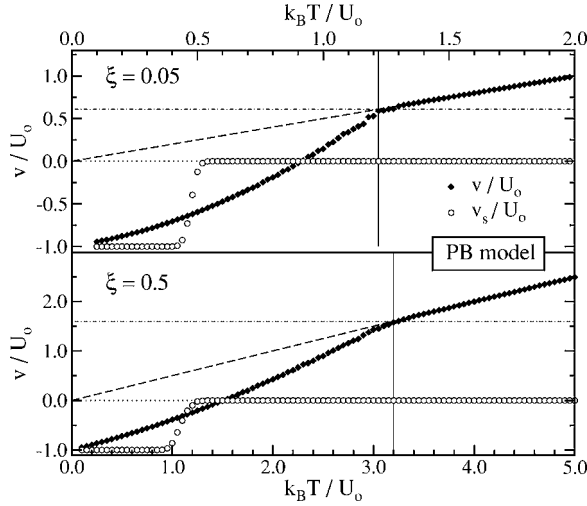
FIG. 7. Temperature dependence (in reduced units $k_B T/U_0$) of the equilibrium potential energy v (full symbols) and energy v_s of underlying saddles (open symbols) for the PB model defined by Eq. (4) with $\xi=0.05$ (upper panel) and $\xi=0.5$ (lower panel). Also indicated in the figure are the values of topological change energy v_θ (horizontal dotted lines), phase transition energy v_c (horizontal dotted-dashed lines) and transition temperature T_c (vertical full line) for $\xi=0.05$ ($v_\theta/U_0=0$, $v_c/U_0 \simeq 0.61$, and $k_B T_c/U_0 \simeq 1.22$) and for $\xi=0.5$ ($v_\theta/U_0=0$, $v_c/U_0 \simeq 1.59$, and $k_B T_c/U_0 \simeq 3.20$). Dashed lines are the T dependence of the potential energy in the high T phase, $v(T)=k_B T/2$.

FIG. 8. Temperature dependence (in reduced units $k_B T/U_0$) of the equilibrium potential energy v (full symbols) and energy v_s of underlying saddles (open symbols) for the SPB model defined by Eq. (5) with $\xi=0.05$ (upper panel) and $\xi=0.5$ (lower panel). Also indicated in the figure is the value of the topological change energy $v_\theta/U_0=0$ (dotted line) for both cases.

results can be used to infer the existence and location of a phase transition. In Fig. 7 we report the temperature dependence of the potential energy per particle $v=V/N$ (full symbols) of the PB model for two different values of ξ, 0.05 (upper panel) and 0.5 (lower panel). Also reported in the figure are the energy v_c (dotted-dashed line) and temperature T_c (full line) of the phase transition point, $v_c/U_0 \simeq 0.61$ and $k_B T_c/U_0 \simeq 1.22$ for $\xi=0.05$, $v_c/U_0 \simeq 1.59$ and $k_B T_c/U_0 \simeq 3.20$ for $\xi=0.5$. Dashed lines are the T dependence of the potential energy in the high T phase, $v(T)=k_B T/2$.

B. Topology

The topology of the Peyrard-Bishop model is studied in the paper of Grinza and Mossa [12]. A topological change is found at the energy value $v_\theta=0$, corresponding to a topological change in the hypersurfaces Σ_v varying v, from a close hypersurface for $v<v_\theta$ to an open one for $v \geqslant v_\theta$ [12]. In Fig. 7 the value of v_θ is indicated by a horizontal dotted line. We note that, also in this case, the topological discontinuity is lower in energy than the thermodynamic one, $v_c>v_\theta$.

V. SYMMETRIC PEYRARD-BISHOP MODEL

A. Thermodynamics

The symmetric Peyrard-Bishop model defined by Eqs. (3) and (5) does not exhibit phase transition at finite T. This can be viewed from the fact that there is always a bound state in the corresponding quantum problem, in analogy with the nonconfined Burkhardt model [23,27]. In Fig. 8 the same
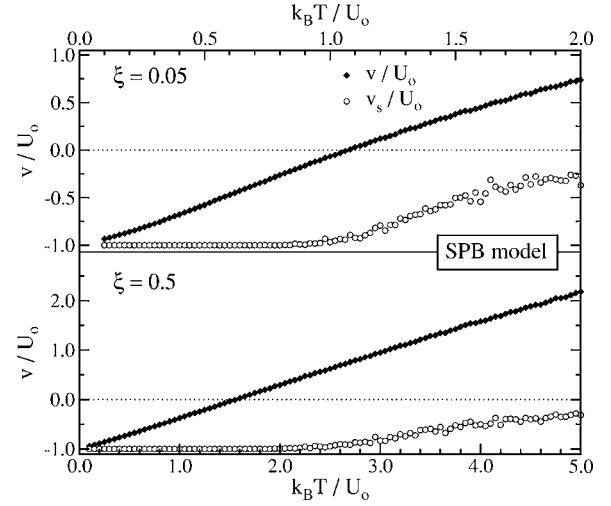
quantities as in the PB case are reported for the SPB model, energy v (full symbols) for $\xi=0.05$ (upper panel) and $\xi=0.05$ (lower panel). It is evident in this case the absence of a phase transition at finite T (in the T-range investigated).

B. Topology

Following a similar argument as in Ref. [11], one can see that also in the SPB case one has a topological change at exactly the same energy level as in the PB model $v_\theta=0$ (even if not identical in strength to the previous one). We refer to the papers in Refs. [11,12] for a more detailed discussion of the topology. In Fig. 8 the value of v_θ is indicated by a horizontal dotted line.

VI. UNDERLYING SADDLES

In this section we study the properties of the stationary points visited by the systems. The concept of "*underlying saddles*" was first introduced in the study of glassy disordered systems [15,16,18] to better understand the topological counterpart of the dynamic transition taking place in these systems. Recently, it has been applied also in the analysis of models that exhibit thermodynamic phase transitions, in order to emphasize the role of topological changes at the "*underlying saddles*" energy in driving the phase transition [8–10].

Here we apply the same methodology to investigate the one-dimensional systems introduced before. Let us start with the models having a continuous potential energy function, the PB and SPB models, which allow for the usual definition of stationary points. At the end of the section we will extend the argument to the discontinuous case of the Burkhardt model.
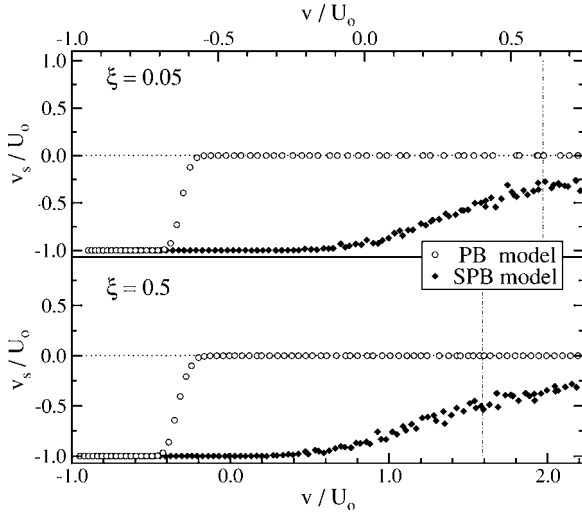
FIG. 9. Map $\mathcal{M}: v \rightarrow v_s$ defined minimizing the pseudopotential $W = |\nabla V|^2$ in the PB and SPB models for $\xi = 0.05$ (upper panel) and $\xi = 0.5$ (lower panel). Also reported are the corresponding v_θ (dotted lines) and v_c (dotted-dashed lines) for $\xi = 0.05$ ($v_\theta = 0, v_c \simeq 0.61$) and $\xi = 0.5$ ($v_\theta = 0, v_c \simeq 1.59$), evidencing the identity $\mathcal{M}(v_c) = v_\theta$.

A. Peyrard-Bishop and symmetric Peyrard-Bishop models

There are only two stationary points in the potential energy hypersurface of both models, a minimum located at $q_1 = q_2 = \cdots = q_N = 0$ and a saddle (with degenerate Hessian matrix) at $q_1 = q_2 = \cdots = q_N = \infty$ [12]. In order to associate one of the two stationary points to each instantaneous configuration of the system, we used a similar trick as in the analysis of glassy systems [15] or mean-field models [8–10]. In the latter one minimized the pseudopotential $W = |\nabla V|^2$ during the dynamic evolution at different temperatures, so introducing a map from equilibrium energy levels to saddle energy levels, $\mathcal{M}: v \rightarrow \mathcal{M}(v) \equiv v_s$. Due to the peculiarity of the present models, where the saddle point is "infinitely" far from each equilibrium configuration, we decided to apply the W minimization method in a two step procedure, (i) first we minimized the W_{int} quantity defined using the interaction potential part of V, $W_{\text{int}} = |\nabla V_{\text{int}}|^2$, where $V_{\text{int}} = \Sigma_{i=1}^{N}(K/2)(q_{i+1} - q_i)^2$; (ii) then we minimized the W_p defined using the on site potential $W_p = |\nabla V_p^{(2,3)}|^2$. This procedure ensures that the point reached is a true stationary point, i.e., the minimum or the saddle. Obviously, this is a quite arbitrary definition of basins of attraction of stationary points. As said in the introduction, the robustness of the results with respect to the possible choices of definition of a saddle basin of attraction is still an open problem.

In Fig. 7 the temperature dependence of the energy v_s (open symbols) of underlying saddles is shown for the case $\xi = 0.05$ (upper panel) and $\xi = 0.5$ (lower panel) in the PB model. The remarkable fact is that at T_c (vertical full line in Fig. 7) the identity $v_s = v_\theta$ holds. The map $\mathcal{M}(v)$ is shown for the PB model (open symbols) in Fig. 9 for the two cases $\xi = 0.05$ (upper panel) and $\xi = 0.5$ (lower panel). One observes that, as pointed out, one has $\mathcal{M}(v_c) = v_\theta$ for both ξ values. The fact that $v_s(T)$ in Fig. 7, as well as $\mathcal{M}(v)$ in Fig. 9, has a "smooth" transition between its low T (or v) and high T

(high v) regions is most likely due to a finite size effect ($N = 500$ here) and both $v_s(T)$ and $\mathcal{M}(v)$ will probably tend towards a step function in the thermodynamic limit. The previous finding indicates that the relevant quantity to consider when we are looking for topological changes related to a phase transition is the underlying stationary point energy, obtained trough a map from the critical level v_c. It is worth noting that the map $\mathcal{M}$ is constant [$\mathcal{M}(v) = v_\theta$] for a broad range of values, also below v_c, at variance with other cases where around the transition point the properties of visited saddles change [7–10]. One can conjecture that the flatness of $\mathcal{M}(v)$ is a pathology of these one-dimensional models, that have a number of stationary points that is not extensive in N (actually there are only two stationary points).

In Fig. 8 we report the same quantities v_s as before (open symbols), now for the SPB model, with $\xi = 0.05$ (upper panel) and $\xi = 0.5$ (lower panel). In this case no phase transition is present, and indeed the topological singularity is never visited, $v_s(T) < v_\theta$ for each finite temperature ($T < \infty$).

B. Burkhardt model

To apply the analysis of the preceding section also to the Burkhardt model, one must find a suitable definition of "saddles" and of "basin of attraction of a saddle" for a discontinuous potential. One possibility is the following: we first minimize the interaction potential $V_{\text{int}} = \Sigma_{i=1}^{N} K|q_{i+1} - q_i|$, which is equivalent to set all the q_i equal to the center of mass coordinate $\bar{q} = N^{-1}\Sigma_i q_i$. If $\bar{q}$ lies in the well of the potential, i.e., $\bar{q} \in [L, L+R]$, we will associate the "minimum" to the initial configuration, otherwise we will associate it to the "saddle" (we use this terminology by analogy with the PB model). It is clear that the average energy of the "underlying saddles" is simply the average of the on-site energy of the center of mass coordinate,

$$v_s(T) = \langle V_p^{(1)}(\bar{q}) \rangle_T. \qquad (29)$$

In the thermodynamic limit the center of mass $\bar{q}$ is peaked around its mean value and then we can substitute the right-hand side of Eq. (29) with $V_p^{(1)}(\langle \bar{q} \rangle)$, a quantity that can be explicitly computed. To determine $\langle \bar{q} \rangle$ we can use the distribution probability $|\phi(x)|^2$, where $\phi(x) = e^{-\beta V_p(x)/2} \psi(x)$ and $\psi(x)$ is the eigenfunction of the transfer matrix operator corresponding to the maximum eigenvalue [23] (see Sec. II A). We note that the saddle energy $v_s(T)$ is a step function, equals the minimum energy $-U_0$ when $\langle \bar{q} \rangle$ lies inside the square well and equals the saddle energy 0 otherwise. The temperature T_J at which the visited "underlying saddle" jumps from minimum to saddle is shown in Fig. 3 (dashed line) as a function of the parameter ξ for the $\zeta = 0$ case. It is worth noting that the temperature T_J lies always below the thermodynamic transition temperature T_c (in analogy with the PB model, see Fig. 7). The same happens for all values of ξ. Therefore, also for the Burkhardt case, at the transition temperature T_c the "underlying saddles" lie at an energy equal to the topological discontinuity energy v_θ, i.e., $\mathcal{M}(v_c) = v_\theta$.

VII. CONCLUSIONS

Studying two particular one-dimensional models discussed in the recent literature [11,12] (Burkhardt model in the confining and nonconfining version, Peyrard-Bishop model and its nonconfining counterpart), we have focused on the relationship between phase transitions and topological changes, recently proposed in the literature [2–5]. In these models, a topological singularity at a given energy value $v_\theta(=0)$ is always found; however, (i) in the confining version a phase transition is found but the critical energy is $v_c > v_\theta$ [12]; (ii) in their nonconfining version there is no phase transition at any finite temperature [11].

These results generated confusion as (i) was interpreted as a confirmation of the *strong topological hypothesis* of Pettini *et al.* [22] while (ii) was considered as an evidence for the unattainability of a purely topological criterion for detecting phase transitions, although demonstrated only for the particular nonconfining one-dimensional models.

Exploiting the concept of "*underlying stationary points*" defined through a generalization of the methods used in the glassy literature (minimization of the pseudopotential $W = |\nabla V|^2$), we have defined a map $\mathcal{M}: v \rightarrow v_s$ from energy level v of V to stationary points, with energy v_s. We have shown that (i) in the confining case, where the phase transition is present, one has $\mathcal{M}(v_c) = v_\theta$, in agreement with the *weak topological hypothesis*; (ii) in the nonconfining case, where the phase transition is not present at finite temperature (as the transition temperature goes continuously to infinity when the confining wall is removed) the energy of the underlying saddles is always *below* the topological singularity, i.e., $v_s(T) < v_\theta, \forall T$; the singular point v_θ is indeed visited for $T \rightarrow \infty$, consistently with the observation that the critical temperature is "infinite" in the nonconfining case.

The *weak topological hypothesis* appears as a possible framework to fit the results that recently appeared in the literature on all the different models investigated so far. Within this hypothesis three different scenarios are possible.

(1) If there is no topological singularity v_θ, a phase transition is not possible; this is consistent with the hypothesis of Pettini *et al.*, topological singularities are *necessary* conditions for a phase transition to take place.

(2) If there is a topological singularity at energy v_θ, a phase transition is also present *if and only if* there exist a temperature T_c such that $v_s(T_c) = v_\theta$ [or equivalently an energy v_c such that $\mathcal{M}(v_c) = v_\theta$].

The above findings seem to indicate that, at least for the particular models investigated, a sufficiency criterion for the phase transition to take place requires the introduction of a statistical measure, thus, we believe that the statement of Kastner [11] concerning the unattainability of a purely topological criterion for detecting phase transitions is indeed correct, even though in Ref. [11] it has been derived using a "borderline" model (see Sec. III C).

Let us conclude with two remarks, (i) as already stated, the definition of the map $\mathcal{M}$ is not unique, different definitions giving (slightly) different results. Thus, the *weak topological hypothesis* contains in its formulation an ambiguity and must be regarded only as a *practical* tool, at least at this stage of comprehension; (ii) nevertheless, we hope that this approach can be of interest for the numerical investigation of systems of "mesoscopic" size (e.g., proteins and large molecules), i.e., such that the number of degrees of freedom is not large enough to allow to detect the presence of a phase transition using standard techniques.

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