On the origin of phase transitions in the absence of symmetry-breaking

On the origin of Phase Transitions in the absence of Symmetry-Breaking

Giulio Pettini,[1,*] Matteo Gori,[2,†] Roberto Franzosi,[3,‡] Cecilia Clementi,[4,§] and Marco Pettini[2,¶]

[1] *Dipartimento di Fisica Università di Firenze, and I.N.F.N., Sezione di Firenze, via G. Sansone 1, I-50019 Sesto Fiorentino, Italy*

[2] *Centre de Physique Théorique, Aix-Marseille University, Campus de Luminy, Case 907, 13288 Marseille Cedex 09, France*

[3] *QSTAR & CNR - Istituto Nazionale di Ottica, Largo Enrico Fermi 2, I-50125 Firenze, Italy*

[4] *Department of Chemistry, Rice University, 6100 Main street, Houston, TX 77005-1892, USA*

(Dated: June 15, 2019)

Abstract

In this paper we investigate the Hamiltonian dynamics of a lattice gauge model in three spatial dimensions. Our model Hamiltonian is defined on the basis of a continuum version of a duality transformation of a three dimensional Ising model. The system so obtained undergoes a thermodynamic phase transition in the absence of a global symmetry-breaking and thus in the absence of an order parameter. It is found that the first order phase transition undergone by this model fits into a microcanonical version of an Ehrenfest-like classification of phase transitions applied to the configurational entropy. It is discussed why the seemingly divergent behaviour of the third derivative of configurational entropy is the effect of a deeper geometrical transition of the equipotential submanifolds of configuration space, which, in its turn, is likely to be the "shadow" of an even deeper transition of topological kind.

Keywords: microcanonical phase transitions; topology and phase transitions; Hamiltonian dynamics and phase transitions

PACS numbers: 05.45.+b; 02.40.-k; 05.20.-y

* pettini@fi.unifi.it

† gori6matteo@gmail.com

‡ roberto.franzosi@ino.it

§ cecilia@rice.edu

¶ pettini@cpt.univ-mrs.fr

I. INTRODUCTION

One of the main topics in Statistical Mechanics concerns phase transitions phenomena. From the theoretical viewpoint, understanding their origin, and the way of classifying them, is of central interest.

Usually, phase transitions are associated with a spontaneous symmetry-breaking phenomenon: at low temperatures the accessible states of a system can lack some of the global symmetries of the Hamiltonian, so that the corresponding phase is the less symmetric one, whereas at higher temperatures the thermal fluctuations allow the access to a wider range of energy states having all the symmetries of the Hamiltonian. In the symmetry-breaking phenomena, the extra variable which characterizes the physical states of a system is the order parameter. The order parameter vanishes in the symmetric phase and is different from zero in the broken-symmetry phase. This is the essence of Landau's theory. If G_0 is the global symmetry group of the Hamiltonian, the order of a phase transition is determined by the index of the subgroup $\mathcal{G} \subset G_0$ of the broken symmetry phase. The corresponding mechanism in quantum field theory is described by the Nambu-Goldstone's Theorem.

However, this is not an all-encompassing theory. In fact, many systems do not fit in this scheme and undergo a phase transition in the absence of a symmetry-breaking. This is the case of liquid-gas transitions, Kosterlitz-Thouless transitions, coulombian/confined regime transition for gauge theories on lattice, transitions in glasses and supercooled liquids, in general, transitions in amorphous and disordered systems, folding transitions in homopolymers and proteins, to quote remarkable examples. All these physical systems lack an order parameter.

Moreover, classical theories, as those of Yang-Lee [2] and of Dobrushin-Lanford-Ruelle [3], require the $N \to \infty$ limit (thermodynamic limit) to mathematically describe a phase transition, but the study of transitional phenomena in finite N systems is particularly relevant in many other contemporary problems [4], for instance related with polymers thermodynamics and biophysics [5], with Bose-Einstein condensation, Dicke's superradiance in microlasers, nuclear physics [6], superconductive transitions in small metallic objects. The topological theory of phase transitions provides a natural framework to get rid of the thermodynamic limit dogma because clear topological signatures of phase transitions are found already at finite and small N [7, 13].

Therefore, looking for generalisations of the existing theories is a well motivated and timely purpose. The present paper aims at giving a contribution in this direction along a line of thought initiated several years ago with the investigation of the Hamiltonian dynamical counterpart of phase transitions [7–9] which eventually led to formulate a topological hypothesis. In fact, Hamiltonian flows ($\mathcal{H}$-flows) can be seen as geodesic flows on suitable Riemannian manifolds [7, 10], and then the question naturally arises of whether and how these manifolds "encode" the fact that their geodesic flows/$\mathcal{H}$-flows are associated or not with a thermodynamic phase transition (TDPT). It is by following this conceptual pathway that one is eventually led to hypothesize that suitable topological changes of certain submanifolds of phase space are the deep origin of TDPT. This hypothesis was corroborated by several studies on specific exactly solvable models [11–15] and by two theorems. These theorems, even if still somewhat controversial [16], state that the unbounded growth with N of relevant thermodynamic quantities, eventually leading to singularities in the $N \to \infty$ limit - the hallmark of an equilibrium phase transition - is *necessarily* due to appropriate topological transitions in configuration space [7, 17–19].

Hence, and more precisely, the present paper aims at investigating whether also TDPT occurring in the absence of symmetry-breaking, and thus in the absence of an order parameter, can be ascribed to some major geometrical change of the previously mentioned manifolds, possibly rooted in a deeper topological change of these same manifolds.

To this purpose, inspired by the dual Ising model, we define a continuous variables Hamiltonian in three spatial dimensions (3D) having the same local (gauge) symmetry of the dual Ising model (reported in Section II) and then proceed to its numerical investigation. The results are reported and discussed in Section III. Through a standard analysis of thermodynamic observables, it is found that this model undergoes a first order phase transition. It is also found that the larger the number of degrees of freedom the sharper the jump of the second derivative of configurational entropy, what naturally fits into a proposed microcanonical version of an Ehrenfest-like classification of phase transitions.

A crucial finding of the present work consists of the observation that this jump of the second derivative of configurational entropy coincides with a jump of the second derivative of a geometric quantity measuring the total dispersion of the principal curvatures of certain submanifolds (the potential level sets) of configuration space. This is a highly non trivial fact because the peculiar energy variation of the geometry of these submanifolds, entailing the jump of the second derivative of the total dispersion of their principal curvatures, is a primitive, a fundamental phenomenon: it is the *cause and not the effect* of the energy dependence of the entropy and its derivatives, that is, the phase transition is a consequence of a deeper phenomenon. In its turn, the peculiar energy-pattern of this geometric quantity appears to be rooted in the variations of topology of the potential level sets, thus the present results provide a further argument in favour of the topological theory of phase transitions, also in the absence of symmetry-breaking.

II. THE MODEL

Starting from the Ising Hamiltonian

$$V_{\text{ising}}\left(\{\sigma_{\mathbf{i}}\}_{\mathbf{i}\in\Lambda}\right) = -J \sum_{\langle\mathbf{ij}\rangle\in\Lambda} \sigma_{\mathbf{i}}\sigma_{\mathbf{j}} \tag{1}$$

with nearest-neighbor interactions ($\langle\mathbf{ij}\rangle$) on a 3D-lattice Λ, where the $\sigma_{\mathbf{i}}$ are discrete dichotomic variables ($\sigma_{\mathbf{i}} = \pm 1$) defined on the lattice sites and J is real positive (ferromagnetic coupling), one defines the potential energy of the dual model [20]

$$V_{\text{dual}}(U) = -J \sum_{\square} U_{\mathbf{ij}}U_{\mathbf{jk}}U_{\mathbf{kl}}U_{\mathbf{li}} \tag{2}$$

where the discrete variables $U_{\mathbf{mm'}}$ are defined on the links joining the sites $\mathbf{m}$ and $\mathbf{m'}$, and $U_{\mathbf{mm'}} = \pm 1$. The summation is carried over all the minimal plaquettes (denoted by $\square$) into which the lattice can be decomposed. The dual model in (2) has the local (gauge) symmetry

$$U_{\mathbf{ij}} \to \varepsilon_{\mathbf{i}}\varepsilon_{\mathbf{j}}U_{\mathbf{ij}} \tag{3}$$

with $\varepsilon_{\mathbf{i}}, \varepsilon_{\mathbf{j}} = \pm 1$, and $\mathbf{i}, \mathbf{j} \in \Lambda$. Such a gauge transformation leaves the model (2) unaltered, and after the Elitzur theorem [21] $\langle U_{\mathbf{ij}}\rangle$ does not qualify as a good order parameter to detect the occurrence of a phase transition because $\langle U_{\mathbf{ij}}\rangle = 0$ always. In other words, no bifurcation of $\langle U_{\mathbf{ij}}\rangle$ can be observed at any phase transition point inherited by the model (2) from the Ising model (1).

In order to define a Hamiltonian flow with the same property of local symmetry – hindering the existence of a standard order parameter – we borrow the analytic form of (2) and replace the discrete dichotomic variables $U_{\mathbf{ij}}$ with continuous ones $U_{\mathbf{ij}} \in \mathbb{R}$. We remark that we donot want to investigate the dual-Ising model, rather we just heuristically refer to it in order to define a gauge model with the desired properties.

Moreover, we add to the continuous version of (2) a stabilizing term which is invariant under the same local gauge transformation (3); this reads

$$V_{\rm quartic}(U) = \alpha \sum_{\langle \mathbf{ij} \rangle} \left(U^2_{\mathbf{ij}} - 1\right)^4 \ , \tag{4}$$

where $\langle \mathbf{ij} \rangle$ stands for nearest-neighbor interactions for link variables and α is a real positive coupling constant.

On a 3D-lattice Λ, and with $I = \{(1,0,0),(0,1,0),(0,0,1)\}$, we thus define the following model Hamiltonian

$$\begin{aligned}\mathcal{H}(\pi, U) =& K(\pi) + V_{\rm ising}(U) + V_{\rm quartic}(U) = \\ =& \sum_{\mathbf{i}\in\Lambda} \sum_{\mu\in I} \frac{1}{2}\pi^2_{\mathbf{i}\mu} - J \sum_{\square\in\Lambda} U_{\mathbf{ij}}U_{\mathbf{jk}}U_{\mathbf{kl}}U_{\mathbf{li}} + \alpha \sum_{\mathbf{i}\in\Lambda} \sum_{\mu\in I} \left(U^2_{\mathbf{i}\mu} - 1\right)^4\end{aligned} \tag{5}$$

whose flow is investigated through the numerical integration of the corresponding Hamilton equations of motion.

A more explicit form of (5) is given by

$$\begin{aligned}\mathcal{H}(\pi, U) = \sum_{i,j,k=1}^{n} \sum_{\nu=1}^{3} \frac{1}{2}\pi^2_{ijk\nu} - J \sum_{i,j,k=1}^{n} [U_{ijk1}U_{i+1jk2}U_{ij+1k1}U_{ijk2} \\ + U_{ijk2}U_{ij+1k3}U_{ijk+12}U_{ijk3} + U_{ijk3}U_{ijk+11}U_{i+1jk3}U_{ijk1}] + \alpha \sum_{i,j,k=1}^{n} \sum_{\nu=1}^{3} \left(U^2_{ijk\nu} - 1\right)^4 ,\end{aligned} \tag{6}$$

where the summation is carried over trihedrals made of three orthogonal plaquettes. Here U_{ijk1} is the link variable joining the sites (i,j,k) and $(i+1,j,k)$, U_{ijk2} is the link variable joining the sites (i,j,k) and $(i,j+1,k)$, U_{ijk3} is the link variable joining the sites (i,j,k) and $(i,j,k+1)$. Similarly, for example, U_{i+1jk2} joins the sites $(i+1,j,k)$ and $(i+1,j+1,k)$, U_{ij+1k1} joins $(i+1,j+1,k)$ and $(i,j+1,k)$, and so on. That is to say that the fourth index labels the direction, i.e which index is varied by one unit.

The Hamilton equations of motion are given by

$$\begin{aligned}\dot{U}_{ijk\nu} &= \pi_{ijk\nu}, \\ \dot{\pi}_{ijk\nu} &= -\frac{\partial \mathcal{H}}{\partial U_{ijk\nu}} \ , \qquad i,j,k = 1,\dots,n; \quad \nu = 1,2,3,\end{aligned} \tag{7}$$

periodic boundary conditions are always assumed.

The numerical integration of these equations is correctly performed only by means of symplectic integration schemes. These algorithms satisfy energy conservation (with zero mean fluctuations around a reference value of the energy) for arbitrarily long times as well as the conservation of all the Poincaré invariants, which include the phase space volume, so that also Liouville's theorem is satisfied by a symplectic integration. We adopted a third-order bilateral symplectic algorithm as described in [22]. We used $J = 1$ and $\alpha = 1$, the integration time step Δt varied from 0.005 at low energy to 0.001 at high energy so as to keep the relative energy fluctuations $\Delta E/E$ close to 10^{-6}.

III. DEFINITION OF THE OBSERVABLES AND NUMERICAL INVESTIGATION

Given any observable $A = A(\pi, U)$, one computes its time average as

$$\langle A\rangle_t = \frac{1}{t}\int_0^t d\tau\ A[\pi(\tau), U(\tau)] \tag{8}$$

along the numerically computed phase space trajectories. For sufficiently long integration times, and for generic nonlinear (chaotic) systems, these time averages are used as estimates of microcanonical ensemble averages in all the expressions given below.

A. Thermodynamic observables

The basic macroscopic thermodynamic observable is temperature. The microcanonical definition of temperature depends on entropy — the basic thermodynamic potential in the microcanonical ensemble — according to the relation

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{\mathcal{V}} , \tag{9}$$

where $\mathcal{V}$ is the volume, E is the energy and the entropy S is given by

$$S(N, E, \mathcal{V}) = k_{\rm B} \log \int d\pi_1 \cdots d\pi_N dU_1 \cdots dU_N\ \delta[E - \mathcal{H}(\pi, U)] \tag{10}$$

where N is the total number of degrees of freedom, $N = 3n^3$ in the present context, and U_k stands for any suitable labelling of them. By means of a Laplace transform technique [23], from Eqs. (9) and (10) one gets (setting $k_{\rm B} = 1$)

$$T = 2\left[(N-2)\langle K^{-1}\rangle\right]^{-1} . \tag{11}$$

where $\langle K^{-1}\rangle$ is the microcanonical ensemble average of the inverse of the kinetic energy $K = E - V(U)$, where $V(U)$ is the potential part of the Hamiltonian (7).

In numerical simulations

$$\langle K^{-1}\rangle = \frac{1}{t}\int_0^t d\tau \, \left[\sum_{i,j,k=1}^{n}\sum_{\nu=1}^{3}\frac{1}{2}\pi^2_{ijk\nu}(\tau)\right]^{-1} . \tag{12}$$

For t sufficiently large $\langle K^{-1}\rangle$ attains a stable value (in general this is a rapidly converging quantity entailing a rapid convergence of T).

Since the invariant measure for nonintegrable Hamiltonian dynamics is the microcanonical measure in phase space, the occurrence of equilibrium phase transitions can be investigated in the microcanonical statistical ensemble through Hamiltonian dynamics [7, 24]. Standard numerical signatures of phase transitions (also found with canonical Monte Carlo random walks in phase space) are: the bifurcation of the order parameter at the transition point (somewhat smoothed at finite number of degrees of freedom), and sharp peaks – of increasing height with an increasing number of degrees of freedom – of the specific heat at the transition point. As already remarked above, our model (7), because of the local (gauge) symmetry, lacks a standard definition of an order parameter as is usually given in the case of symmetry-breaking phase transitions. And in fact, in every numerical simulation of the dynamics we have computed the time average $\langle\langle U_{\mathbf{ij}}\rangle\rangle_t$ always finding $\langle\langle U_{\mathbf{ij}}\rangle\rangle_t \simeq 0$ independently of the lattice size and of the energy value (the double average means averaging over the entire lattice first, and then averaging over time).

Thus, the presence of a phase transition is detected through the shape of the so-called caloric curve, that is, $T = T(E)$. For the model in (7) this has been computed by means of Eq. (11). Then the *microcanonical* constant-volume specific heat follows according to the relation $1/C_{\mathcal{V}} = \partial T(E)/\partial E$. The numerical computation of specific heat can be independently performed, with respect to the caloric curve, as follows. Starting with the definition of the entropy, given in (10), an analytic formula can be worked out [23], which is exact at *any* value of N. This formula reads

$$c_{\mathcal{V}}(E) = \frac{C_{\mathcal{V}}}{N} = \frac{N(N-2)}{4}\left[(N-2) - (N-4)\frac{\langle K^{-2}\rangle}{\langle K^{-1}\rangle^2}\right]^{-1} , \tag{13}$$

and this is the natural expression to work out the microcanonical specific heat by means of Hamiltonian dynamical simulations.

In order to get the above defined specific heat, time averages of the kind

$$\langle K^\alpha \rangle_t = \frac{1}{t} \int_0^t d\tau \left[\sum_{i,j,k=1}^{n} \sum_{\nu=1}^{3} \frac{1}{2} \pi_{ijk\nu}^2(\tau) \right]^\alpha$$

are computed with $\alpha = -1, -2$. Then, for sufficiently large t, the microcanonical averages $\langle K^\alpha \rangle$ can be replaced by $\langle K^\alpha \rangle_t$.

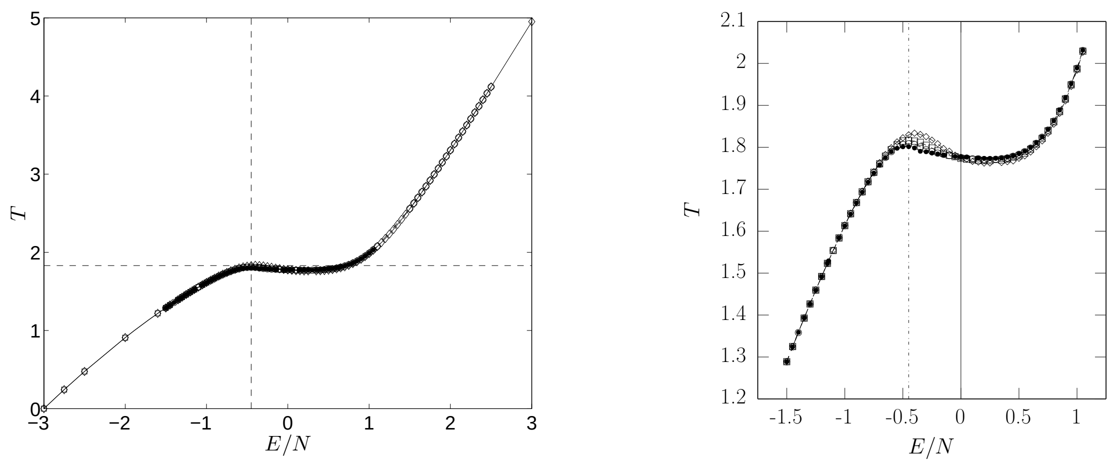

Figure 1. Caloric curve. The temperature, computed according to Eq.(11) is reported versus E/N. Lattice dimensions: $n^3 = 6 \times 6 \times 6$ (rhombs), $n^3 = 8 \times 8 \times 8$ (squares), $n^3 = 10 \times 10 \times 10$ (circles), $n^3 = 14 \times 14 \times 14$ (full circles). The dashed lines identify the point of flat tangency at lower energy. The right panel is a zoom of the central part of the left panel.

In Figure 1 the caloric curve is reported for different sizes of the lattice. A kink, typical of first order phase transitions, can be seen. This entails the presence of negative values of the specific heat, and, consequently, ensemble nonequivalence for the model under consideration. And, in fact, in Figure 2, where we report the outcomes of the computations of the specific heat according to Eq.(13), we can observe an energy interval where the specific heat $C_{\mathcal{V}}$ is negative, and very high peaks are also found. Nevertheless, at this stage these peaks can be attributed only to the existence of two points of flat tangency to the caloric curve and cannot yet be attributed to an analyticity loss of the entropy (see Section III C).

In Figure 3 the average potential energy per lattice site $u = \langle V \rangle / N$ is displayed as a function of the total energy density. Also in this case we observe a regular function which is stable with the number of degrees of freedom. The dashed lines identify the phase transition point which corresponds to $E_c/N \simeq -0.45$ and $u_c \simeq -1.32$.

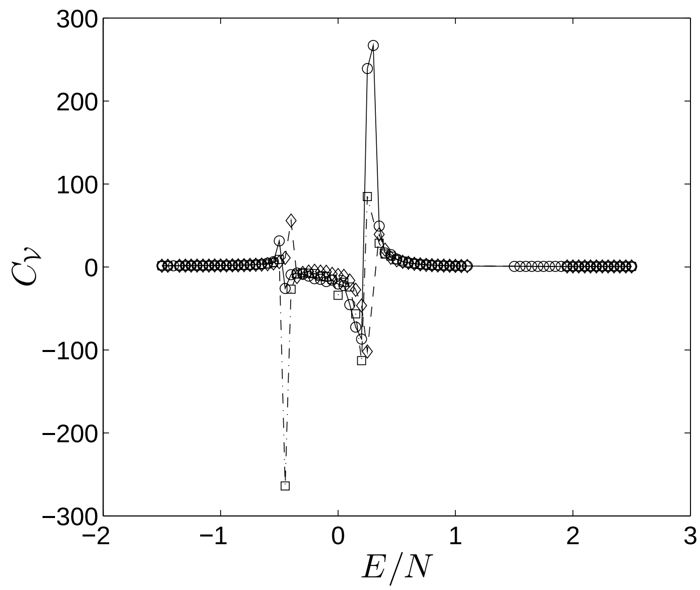

Figure 2. Constant volume specific heat computed by means of Eq.(13). Lattice dimensions: $n^3 = 6 \times 6 \times 6$ (rhombs), $n^3 = 8 \times 8 \times 8$ (squares), $n^3 = 10 \times 10 \times 10$ (circles).

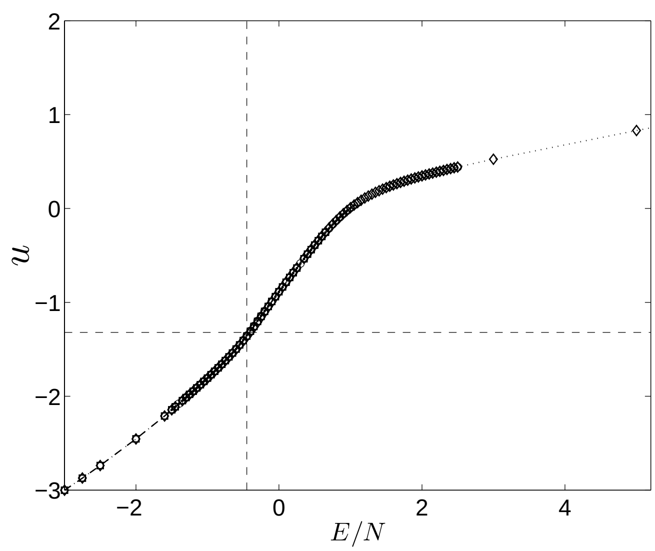

Figure 3. Internal potential energy density computed through Eq.(8) where the observable A is the potential function per degree of freedom of the system. Lattice dimensions: $n^3 = 6 \times 6 \times 6$ (rhombs), $n^3 = 8 \times 8 \times 8$ (squares), $n^3 = 10 \times 10 \times 10$ (circles). The vertical line at $E \simeq -0.45$ locates the phase transition point, correspondingly, at $u \simeq -1.32$, the critical potential energy density is determined.

The results so far reported provide us with a standard numerical evidence of the existence of a first order phase transition undergone by the model investigated. Besides standard thermodynamic observables, the study of phase transitions through Hamiltonian dynamics makes available a new observable, the largest Lyapunov exponent λ, which is of purely dynamical kind, and which has usually displayed peculiar patterns in presence of a symmetry-breaking phase transition [7, 9, 25, 27–30]. Therefore in the following Section an attempt is made to characterise the phase transition undergone by our model also through the energy dependence of λ.

B. A Dynamic observable: the largest Lyapunov exponent

The largest Lyapounov exponent λ is the standard and most relevant indicator of the dynamical stability/instability (chaos) of phase space trajectories. Let us quickly recall that the numerical computation of λ proceeds by integrating the tangent dynamics equations, which, for Hamiltonian flows, read

$$\begin{aligned} \dot{\xi}_i &= \zeta_i \ , \\ \dot{\zeta}_i &= -\sum_{j=1}^{N} \left(\frac{\partial^2 V}{\partial q_1 \partial q_j} \right)_{q(t)} \xi_j \ , \qquad i = 1, \dots, N \end{aligned} \tag{14}$$

together with the equations of motion of the Hamiltonian system under investigation. Then the largest Lyapunov exponent λ is defined by

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \log \frac{[\xi_1^2(t) + \cdots + \xi_N^2(t) + \zeta_1^2(t) + \cdots + \zeta_N^2(t)]^{1/2}}{[\xi_1^2(0) + \cdots + \xi_N^2(0) + \zeta_1^2(0) + \cdots + \zeta_N^2(0)]^{1/2}} \ , \tag{15}$$

In a numerical computation the discretized version of (15) is used, with $\boldsymbol{\xi} = (\xi_1, \dots, \xi_{2N})$ and $\xi_{i+N} = \dot{\xi}_i$

$$\lambda = \lim_{m\to\infty} \frac{1}{m} \sum_{i=1}^{m} \frac{1}{\Delta t} \log \frac{\|\boldsymbol{\xi}[(i+1)\Delta t]\|}{\|\boldsymbol{\xi}(i\Delta t)\|} \ , \tag{16}$$

where, after a given number of time steps Δt, for practical numerical reasons it is convenient to renormalize the value of $\|\boldsymbol{\xi}\|$ to a fixed one. The numerical estimate of λ is obtained by retaining the time asymptotic value of $\lambda(m\Delta t)$. This is obtained by checking the relaxation pattern of $\log \lambda(m\Delta t)$ versus $\log(m\Delta t)$.

Note that λ can be expressed as the time average of a suitable observable defined as

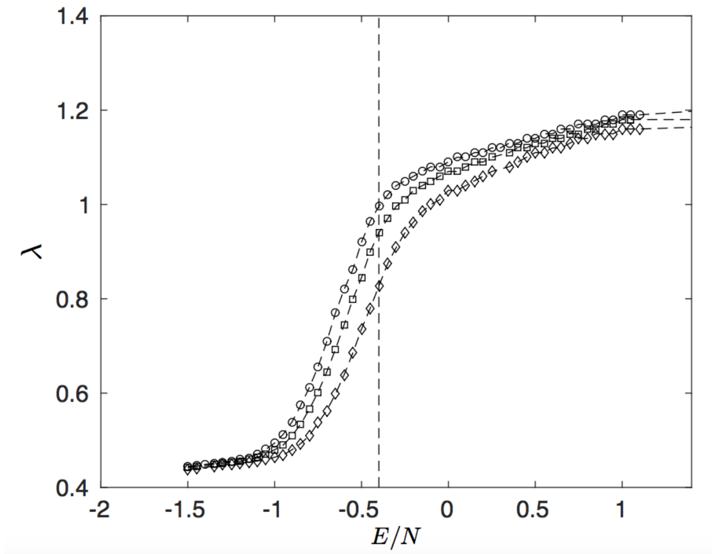

Figure 4. Largest Lyapunov exponent versus the energy per degree of freedom. Lattice dimensions: $n^3 = 6 \times 6 \times 6$ (rhombs), $n^3 = 8 \times 8 \times 8$ (squares), $n^3 = 10 \times 10 \times 10$ (circles). The dashed vertical l line indicates the phase transition point.

follows. From the compact notation

$$\dot{\xi}_i = \sum_k J_{ik}[q(t)]\xi_k$$

for the system (14) and observing that

$$\frac{1}{2}\frac{d}{dt}\log(\xi^T\xi) = \frac{\xi^T\dot{\xi} + \dot{\xi}^T\xi}{2\xi^T\xi} = \frac{\xi^T J[q(t)]\xi + \xi^T J^T[q(t)]\xi}{2\xi^T\xi} ,$$

setting $\mathcal{J}[q(t),\xi(t)] = \{\xi^T J[q(t)]\xi + \xi^T J^T[q(t)]\xi\}/(2\xi^T\xi)$, one gets

$$\lambda = \lim_{t\to\infty}\frac{1}{t}\log\frac{\|\xi(t)\|}{\|\xi(0)\|} = \lim_{t\to\infty}\frac{1}{t}\int_0^t d\tau\, \mathcal{J}[q(\tau),\xi(\tau)] \ , \tag{17}$$

which *formally* gives λ as a time average as per Eq.(8).

The numerical results summarised in Figure 4 qualitatively indicate a transition between two dynamical regimes of chaoticity: from a weakly chaotic dynamics at low energy density values, to a more chaotic dynamics at large energy density values. However the transition between these dynamical states is a mild one. At variance with those models where a phase transition stems from a symmetry-breaking, here there is no peculiar property of the shapes of $\lambda = \lambda(E/N)$ in correspondence of the phase transition. Therefore, in the following Section we directly tackle the numerical study of the differentiability class of the entropy.

C. Microcanonical definition of phase transitions

In recent times, the problem of tackling equilibrium phase transitions in the microcanonical ensemble has attracted increasing interest [4, 31–35], being of fundamental importance in presence of ensemble inequivalence, or in the case of a dynamical approach based on Hamiltonian dynamics, to quote just a few examples. At the end of the present Section, we will take advantage especially of a recent and very interesting proposal in Ref.[35] which, on the one side allows to give a coherent interpretation of our results, and on the other side can be given some complementary support by what will be discussed in the following. Let us begin, however, with a somewhat different/complementary viewpoint. As is well known, according to the Ehrenfest classification, the order of a phase transition is given by the order of the discontinuous derivative with respect to temperature T of the Helmholtz free energy $F(T)$. However, a difficulty arises in presence of divergent specific heat C_V associated with a second order phase transition because this implies a divergence of $(\partial^2 F/\partial T^2)$, and, in turn, a discontinuity of $(\partial F/\partial T)$ so that the distinction between first and second order transitions is lost. By resorting to the concept of symmetry-breaking, Landau theory circumvents this difficulty by classifying the order of a phase transition according to the index of the symmetry group of the broken-symmetry phase which is a subgroup of the group of the more-symmetric phase. As in the present work we are tackling a system undergoing a phase transition in the absence of symmetry-breaking, we have to get back to the origins as follows. According to the Ehrenfest theory, a phase transition is associated with a loss of analyticity of a thermodynamic potential (Helmholtz free energy, or, equivalently Gibbs free energy), and the order of the transition depends on the differentiability class of this thermodynamic potential. Later, on a mathematically rigorous ground, the identification of a phase transition with an analyticity loss of a thermodynamic potential (in the gran-canonical ensemble) was confirmed by the Yang-Lee theorem. Now, let us consider the statistical ensemble which is the natural counterpart of microscopic Hamiltonian dynamics, that is, microcanonical ensemble. As already recalled in Section III.A, here the relevant thermodynamic potential is entropy, and considering the specific heat

$$C_V^{-1} = \frac{\partial T(E)}{\partial E} \qquad \text{which, after Eq.(9), reads} \qquad C_V = -\left(\frac{\partial S}{\partial E}\right)^2 \left(\frac{\partial^2 S}{\partial E^2}\right)^{-1} , \tag{18}$$

from the last expression we see that C_V can diverge only as a consequence of the vanishing of $(\partial^2 S/\partial E^2)$ which a-priori has nothing to do with a loss of analyticity of $S(E)$, as it has been already remarked in Section III.A concerning the peaks of C_V reported in Figure 2. For standard Hamiltonian systems (i.e. quadratic in the momenta) the relevant information is carried by the configurational microcanonical ensemble, where the configurational canonical free energy is

$$f_N(\beta) \equiv f_N(\beta; V_N) = \frac{1}{N} \log \int_{(\Lambda^d)^{\times n}} dq_1 \dots dq_N \;\; \exp[-\beta V_N(q_1, \dots, q_N)]$$

with and the configurational microcanonical entropy (in units s.t. $k_B = 1$) is

$$S_N(\bar{v}) \equiv S_N(\bar{v}; V_N) = \frac{1}{N} \log \int_{(\Lambda^d)^{\times n}} dq_1 \cdots dq_N \;\delta[V_N(q_1, \dots, q_N) - v] \;, \;,$$

where $\bar{v} = v/N$ is the potential energy per degree of freedom, and $\delta[\cdot]$ is the Dirac functional. Then $S_N(\bar{v})$ is related to the configurational canonical free energy, f_N, for any $N \in \mathbb{N}$, $\bar{v} \in \mathbb{R}$, and $\beta \in \mathbb{R}$ through the Legendre transform

$$-f_N(\beta) = \beta \cdot \bar{v}_N - S_N(\bar{v}_N) \tag{19}$$

where the inverse of the configurational temperature $T(v)$ is given by $\beta_N(\bar{v}) = \partial S_N(\bar{v})/\partial \bar{v}$. Then consider the function $\phi(\bar{v}) = f_N[\beta(\bar{v})]$, from $\phi'(\bar{v}) = -\bar{v}\;[d\beta_N(\bar{v})/d\bar{v}]$ we see that if $\beta_N(\bar{v}) \in \mathcal{C}^k(\mathbb{R})$ then also $\phi(\bar{v}) \in \mathcal{C}^k(\mathbb{R})$ which in turn means $S_N(\bar{v}) \in \mathcal{C}^{k+1}(\mathbb{R})$ while $f_N(\beta) \in \mathcal{C}^k(\mathbb{R})$. Hence, if the functions $\{S_N(\bar{v})\}_{N\in\mathbb{N}}$ are convex, thus ensuring the existence of the above Legendre transform, and if in the $N \to \infty$ limit it is $f_\infty(\beta) \in \mathcal{C}^0(\mathbb{R})$ then $S_\infty(\bar{v}) \in \mathcal{C}^1(\mathbb{R})$, and if $f_\infty(\beta) \in \mathcal{C}^1(\mathbb{R})$ then $S_\infty(\bar{v}) \in \mathcal{C}^2(\mathbb{R})$. So far we have seen that, generically (that is apart from any possible counterexample), if $f_N(\beta) \in \mathcal{C}^k(\mathbb{R})$ then $S_N(\bar{v}) \in \mathcal{C}^{k+1}(\mathbb{R})$. This all what is needed to *heuristically* proceed to a classification of phase transitions *à la* Ehrenfest in the present microcanonical configurational context. In fact, the original Ehrenfest definition associates a first or second order phase transition with a discontinuity in the first or second derivatives of $f_\infty(\beta)$, that is with $f_\infty(\beta) \in \mathcal{C}^0(\mathbb{R})$ or $f_\infty(\beta) \in \mathcal{C}^1(\mathbb{R})$, respectively. This premise suggests to associate a first order phase transition with a discontinuity of the second derivative of the entropy $S_\infty(\bar{v})$, and to associate a second order phase transition with a discontinuity of the third derivative of the entropy $S_\infty(\bar{v})$. Let us stress that this definition is proposed regardless the existence of the Legendre transform, which typically fails in presence of first order phase transitions which bring about a kink-shaped energy dependence of the entropy [4]. Thus, strictly speaking, the definition that we are putting forward does not mathematically and logically stem from the original Ehrenfest classification. The introduction of this entropy-based classification of phase transitions *à la* Ehrenfest is *heuristically* motivated, but to some extent arbitrary. Its advantage is that it no longer suffers the previously mentioned difficulty arising in the framework of canonical ensemble, including here both divergent specific heat in presence of a second order phase transition, and ensemble non-equivalence. In the end the usefulness of this classification has to be checked against practical examples. The gauge model, here under investigation, provides a first benchmarking in this direction.

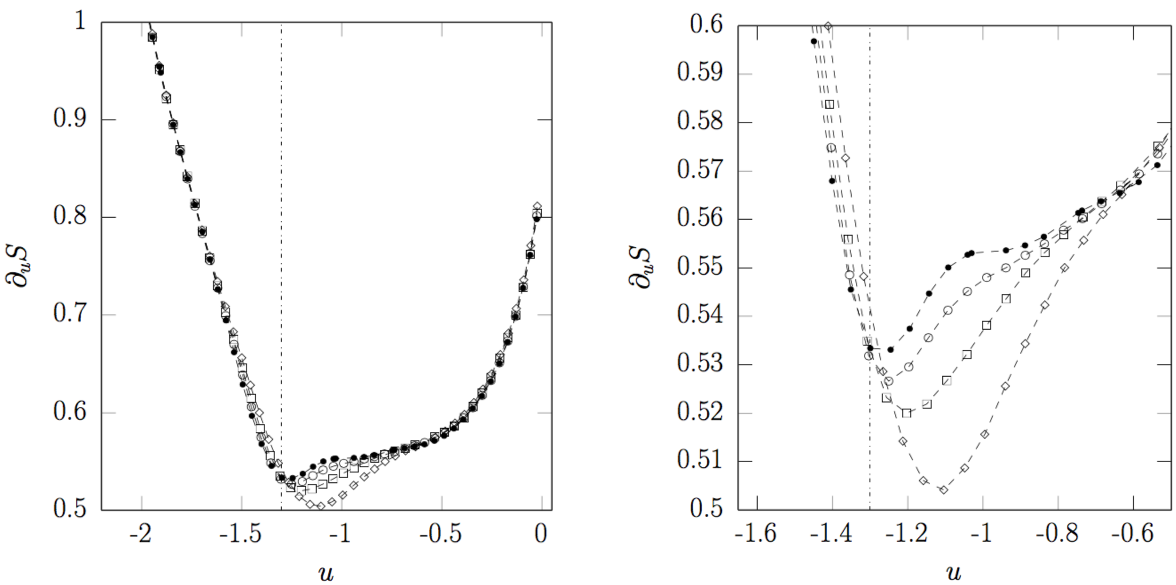

Figure 5. First derivative $\partial S/\partial u$ of the configurational entropy versus the average potential energy per degree of freedom u. Lattice dimensions: $n^3 = 6 \times 6 \times 6$ (red full circles), $n^3 = 8 \times 8 \times 8$ (green full circles), $n^3 = 10 \times 10 \times 10$ (blue full circles), $n^3 = 14 \times 14 \times 14$ (black full circles). The right panel displays a zoom of the transition region. The vertical dot-dashed line locates the phase transition point.

From the numerical results concerning the functions $T(E)$ and $u(E)$, reported in Figure 1 and Figure 3, respectively, we computed the first and second derivatives of the configurational entropy as

$$\frac{\partial S}{\partial u} = \frac{\partial S}{\partial E}\frac{dE}{du} = \frac{1}{T(E)}\frac{dE}{du} , \tag{20}$$

$$\frac{\partial^2 S}{\partial u^2} = \frac{\partial}{\partial u}\left(\frac{1}{T(E)}\frac{dE}{du}\right) . \tag{21}$$

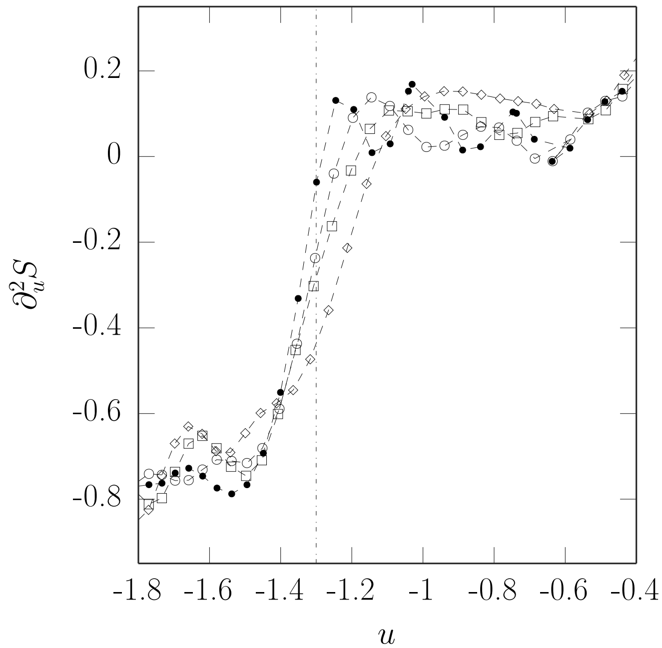

Figure 6. Second derivative $\partial^2 S/\partial u^2$ of the configurational entropy versus the average potential energy per degree of freedom u. Lattice dimensions: $n^3 = 6 \times 6 \times 6$ (rhombs), $n^3 = 8 \times 8 \times 8$ (squares), $n^3 = 10 \times 10 \times 10$ (circles), $n^3 = 14 \times 14 \times 14$ (full circles). The vertical dot-dashed line locates the phase transition point.

The derivative (dE/du) entering Eq.(20) is obtained after inversion of the function $u = u(E)$ reported in Figure 3 and by means of a spline interpolation of its points. Whereas $\partial_u^2 S(u)$ in Eq.(21) is computed from the raw numerical data, and the derivatives with respect to u have been obtained by means of a standard central difference formula.

The four patterns of $\partial_u S(u)$, computed for different sizes of the lattice and reported in Figure 5, show that each $\partial_u S(u)$ appears splitted into two monotonic branches, one decreasing and the other increasing as functions of u, respectively. Approximately out of the interval $u \in (-1.6, -0.65)$ the four patterns are perfectly superposed, whereas within this interval - which contains the transition value $u_c \simeq -1.32$ - we can observe that the transition from $\partial_u S < 0$ to $\partial_u S > 0$ gets sharper at increasing lattice dimension. This means that the second derivative of the entropy, $\partial_u^2 S(u)$, tends to make a sharper jump at increasing N. And in fact, this is what is suggested by the four patterns of $\partial_u^2 S(u)$ - computed for the same sizes of the lattice - reported in Figure 6. These are strongly suggestive to belong to a sequence of patterns converging to a step-like limit pattern. In this case the third order derivative ($\partial^3 S/\partial u^3$) would asymptotically diverge entailing a loss of analyticity of the entropy which, in fact, would drop to $S_\infty(u) \in \mathcal{C}^1$. And this is in agreement with the above proposed classification *à la* Ehrenfest.

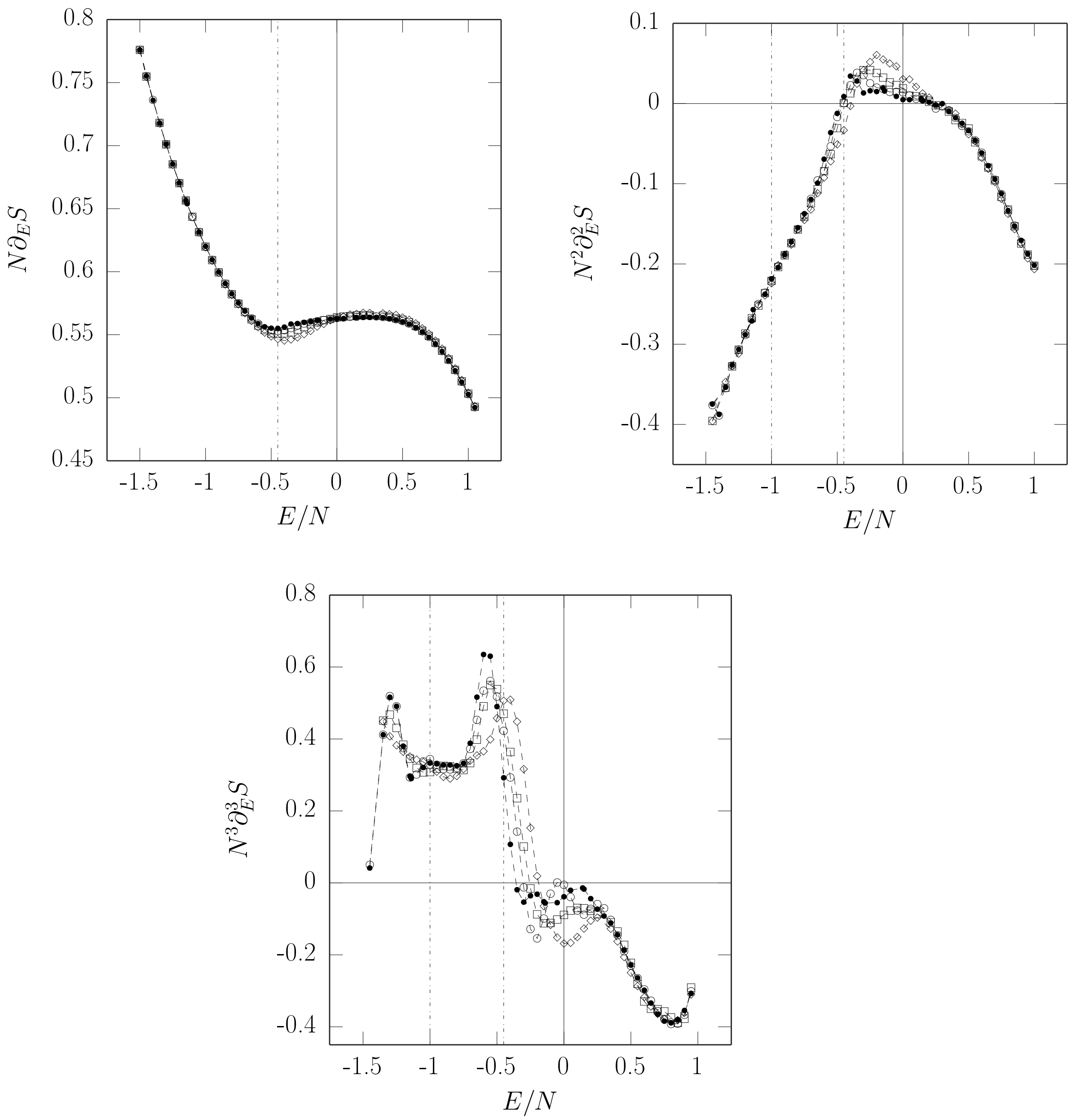

Figure 7. The first three derivatives of the entropy versus energy density E/N. The vertical dot-dashed lines are at $E/N \simeq -0.45$ and at $E/N \simeq -1$. Lattice dimensions: $n^3 = 6\times6\times6$ (rhombs), $n^3 = 8\times8\times8$ (squares), $n^3 = 10\times10\times10$ (circles), $n^3 = 14\times14\times14$ (full circles).

It is worth noting that on the basis of the definition that we have chosen to identify a first order phase transition we have found evidence of only one transition point, despite the presence of two peaks of the specific heat. In fact, only the first peak appears to be related with the tendency to develop a loss of analyticity of the entropy with increasing N. At first sight this is somewhat surprising, but this fact can be understood in the light of Ref.[35] and hence by considering the energy dependence of $(\partial^2 S/\partial E^2)$, reported in Figure 7. Consider the first point where $(\partial^2 S/\partial E^2) = 0$, at $E/N \simeq -1.3$, here we have also $(\partial S/\partial E) > 0$ and $(\partial^3 S/\partial E^3) > 0$ so that, according to the classification given in [35], this corresponds to an *independent* first order transition point, whereas at the second point where $(\partial^2 S/\partial E^2) = 0$, that is at $E/N \simeq 0.3$, we have $(\partial^3 S/\partial E^3) < 0$ and still $(\partial S/\partial E) > 0$ so that this point does not correspond to any kind of phase transition; for this to happen, the first derivative of the entropy had to be negative. In Figure 7 we can identify two other inflection points of the entropy, one is located at $E/N \simeq -1$ for which the third derivative of the entropy has a positive minimum, that is, $(\partial^3 S/\partial E^3) > 0$, $(\partial^4 S/\partial E^4) = 0$, and $(\partial^5 S/\partial E^5) > 0$, which corresponds to an independent third order phase transition. This is a soft transition for which we cannot identify any specific feature in the observables reported in Figures 1,2 and 3, the only clue that we could cautiously recognize in Figure 4, around $E/N \simeq -1$, is that here the largest Lyapunov exponent starts to increase. As far as the second inflection point at $E/N \simeq 0.75$ is concerned, we can see in Figure 7 that $(\partial^3 S/\partial E^3) < 0$, $(\partial^4 S/\partial E^4) = 0$, and $(\partial^5 S/\partial E^5) > 0$, and, according to Ref.[35], this does not correspond to any phase transition point.

Remarkably, for the system that we are considering in the present work which has a thermodynamic limit, the first order *independent* phase transition point corresponds to an asymptotic loss of analyticity of the entropy. It will be worth to further investigate this point in order to figure out whether, for example, this could make a difference between dependent and independent transition points, that is, if independent phase transition points are associated with singularities of the entropy, of course for systems having a thermodynamic limit.

D. A geometric observable for the level sets Σ_v in configuration space

We have seen in the preceding Section that - within the confidence limits of a numerical investigation - the first order phase transition of the gauge model under investigation seems to correspond to an asymptotic divergence of the third derivative $(\partial^3 S/\partial u^3)$ of the microcanonical configurational entropy. The question now is whether this fact can be the "shadow" of a deeper phenomenon, that is, of the occurrence of some major and suitable change of geometrical - and possibly also topological - properties of some subspaces of the configuration space associated with the model. More precisely, and along a geometrical/topological approach already put forward in recent years and summarised in Ref.[7], the relevant information about the appearance of a phase transition in a physical system is already encoded into peculiar changes with v of the geometry and topology of the members of the family of level sets $V_N(q_1,\dots,q_N) = v \in \mathbb{R}$ of its potential function $V(q_1,\dots,q_N)$, equivalently denoted by $\Sigma_v^N = V_N^{-1}(v)$, which are hypersurfaces of configuration space.

Constructively, relevant geometric quantities can be computed through the extrinsic geometry of hypersurfaces of a Euclidean space. To do this one has to study the way in which an N-surface Σ curves around in $\mathbb{R}^{N+1}$ by measuring the way the normal direction changes as we move from point to point on the surface. The rate of change of the normal direction $\mathbf{N}$ at a point $x \in \Sigma$ in direction $\mathbf{v}$ is described by the *shape operator* (sometimes also called Weingarten's map) $L_x(\mathbf{v}) = -\nabla_{\mathbf{v}}\mathbf{N} = -(\mathbf{v}\cdot\nabla)\mathbf{N}$, where $\mathbf{v}$ is a tangent vector at x and $\nabla_{\mathbf{v}}$ is the directional derivative; gradients and vectors being represented in $\mathbb{R}^{N+1}$.

For the level sets of a regular function, as is the case of the constant-energy hypersurfaces in the phase space of Hamiltonian systems or of the equipotential hypersurfaces in configuration space, thus generically defined through a regular real-valued function f as $\Sigma_a := f^{-1}(a)$, the normal vector is $\mathbf{N} = \nabla f/\|\nabla f\|$. The eigenvalues $\kappa_1(x),\dots,\kappa_N(x)$ of the shape operator are the principal curvatures at $x \in \Sigma$. For the potential level sets $\Sigma_v = V^{-1}(v)$ the trace of the shape operator at any given point is the mean curvature at that point and can be written as [7, 36]

$$M = -\frac{1}{N}\nabla\cdot\left(\frac{\nabla V}{\|\nabla V\|}\right) = \frac{1}{N}\sum_{i=1}^{N}\kappa_i \ . \tag{22}$$

We have numerically computed the second moment of M averaged along the Hamiltonian flow

$$\sigma_M = N\langle Var(M)\rangle_t = N[\langle M^2\rangle_t - \langle M\rangle_t^2] \simeq \frac{1}{N}\sum_{i=1}^{N}\langle\kappa_i^2\rangle_t - \frac{1}{N}\sum_{i=1}^{N}\langle\kappa_i\rangle_t^2 \ , \tag{23}$$

where we have assumed that the correlation term $N^{-2}\sum_{i,j}[\langle k_i k_j\rangle_t - \langle k_i\rangle_t\langle k_j\rangle_t]$ vanishes. In fact, on the one side there is no conserved ordering of the eigenvalues of the shape operator along a dynamical trajectory, and on the other side the averages are performed along chaotic trajectories (the largest Lyapounov exponent is always positive) so that k_i and k_j vary almost randomly from point to point and independently one from the other.

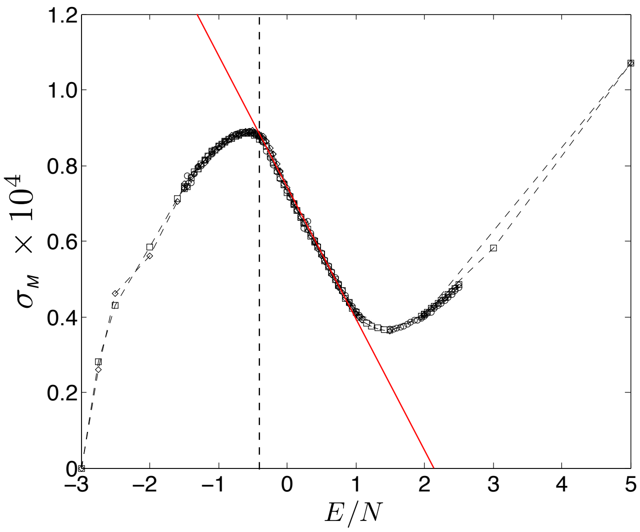

Figure 8. Second moment of the total mean curvature of the potential level sets Σ_u versus energy density E/N. $n^3 = 6 \times 6 \times 6$ (rhombs), $n^3 = 8 \times 8 \times 8$ (squares), $n^3 = 10 \times 10 \times 10$ (circles). The oblique red line is a guide to the eye. The vertical dashed line at $E/N \simeq -0.45$ corresponds to the phase transition point and to the point where the second derivative $d^2\sigma_M/dE^2$ jumps from a negative value to zero.

The numerical results are reported in Figure 8 and Figure 9, where an intriguing feature of the patterns of $\sigma_M(E)$ and $\sigma_M(u)$ is evident: below the transition point (marked with a vertical dashed line) the concavity of both $\sigma_M(E)$ and $\sigma_(u)$ is oriented downward so that $d^2\sigma_M/dE^2$ and $d^2\sigma_M/du^2$ are negative, whereas just above the transition point both $\sigma_M(E)$ and $\sigma_M(u)$ are segments of a straight line, so that $d^2\sigma_M/dE^2$ and $d^2\sigma_M/du^2$ vanish. Thus both derivatives make a jump at the transition point. Again within the validity limits of numerical investigations, this means that the third order derivatives, and in particular $d^3\sigma_M/du^3$, diverge. It is then natural to think of a connection with the asymptotic divergence of d^3S/du^3 suggested by the results reported in the preceding Section.

Remark. There is a point of utmost importance to comment on. In presence of a phase transition (and of a finite size of a phase transition as is the case of numerical simulations) the typical variations of many observables at the transition point are the effects of the singular properties of the statistical measures and hence of the corresponding thermodynamic

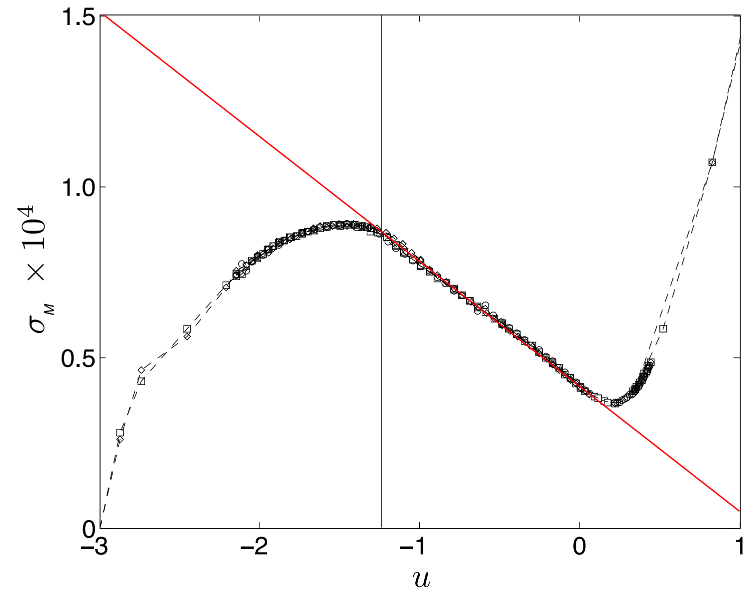

Figure 9. Second moment of the total mean curvature of the potential level sets Σ_u versus the average potential energy per degree of freedom u. $n^3 = 6\times6\times6$ (rhombs), $n^3 = 8\times8\times8$ (squares), $n^3 = 10\times10\times10$ (circles). The oblique red line is a guide to the eye. The vertical blue line at $u \simeq -1.32$ corresponds to the phase transition point and to the point where the second derivative $d^2\sigma_M/du^2$ jumps from a negative value to zero.

potentials (entropy, free energy, pressure). But this is not true for the geometric quantity $\sigma_M(u)$ which is *independent* of the properties of any statistical measure. Peculiar changes of the geometry of the potential level sets of configuration space (detected by σ_M) constitute the deep origin, the *cause* of phase transitions, *not an effect*. The singular pattern of σ_M at the transition point is a primitive phenomenon. In other words, geometrical variations of the spaces where the statistical measures are defined (phase space and configuration space) entail singular properties of these measures [7]. The vice versa is meaningless.

Let us now explore the possibility that the jump of the second derivative of $\sigma_M(u)$ - and consequently the jump of the second derivative of the configurational entropy $S(u)$ - can be both attributed to an even deeper phenomenon: some identifiable change of the topology of the $\{\Sigma_u\}_{u\in\mathbb{R}}$. In what follows, by resorting to the best, non-trivial approximations at present available it is shown that this might well be the case, even if a proof in the strong sense cannot yet be given.

Consider the pointwise dispersion of the principal curvatures

$$s_\kappa = \frac{1}{N}\sum_{i=1}^{N}(\kappa_i - \overline{\kappa})^2 \tag{24}$$

where

$$\overline{\kappa} = \frac{1}{N}\sum_{i=1}^{N}\kappa_i \tag{25}$$

equation (24) is equivalently rewritten as [37]

$$s_\kappa = \frac{1}{N^2}\sum_{i,j=1}^{N}(\kappa_i - \kappa_j)^2 \tag{26}$$

and the time average along the Hamiltonian flow of s_κ is then equivalently written as

$$\langle s_\kappa\rangle_t = \frac{1}{N}\sum_{i=1}^{N}\langle\kappa_i^2\rangle_t - \langle\overline{\kappa}^2\rangle_t = \frac{1}{N^2}\sum_{i,j=1}^{N}\langle(\kappa_i - \kappa_j)^2\rangle_t \ . \tag{27}$$

Now, from Eqs.(23) and (27) we get

$$\sigma_M - \langle s_\kappa\rangle_t \simeq -\frac{1}{N}\sum_{i=1}^{N}\langle\kappa_i\rangle_t^2 + \langle\overline{\kappa}^2\rangle_t \tag{28}$$

so that, based on the empirical/numerical observation that at large N the potential level sets locally appear as of almost constant curvature, that is, locally isotropic, we make a "quasi isotropy" assumption which is equivalent to replace the κ_i with their average $\overline{\kappa}$ in the first term of the r.h.s. of (28), hence it follows $\sigma_M - \langle s_\kappa\rangle_t \simeq -\langle\overline{\kappa}\rangle_t^2 + \langle\overline{\kappa}^2\rangle_t$, and as $\overline{\kappa}$ in Eq.(25) is the same of M in Eq.(22) one trivially gets

$$(1 - \frac{1}{N})\sigma_M - \langle s_\kappa\rangle_t \simeq 0 \tag{29}$$

so that, under this "quasi isotropy" assumption, σ_M in Eq.(23) can be used to estimate $\langle s_\kappa\rangle_t$. Then, as the ergodic invariant measure of chaotic Hamiltonian dynamics is the microcanonical one, the time averages $\langle\cdot\rangle_t$ provide the values of the surface averages $\langle\cdot\rangle_{\Sigma_E}$. Hence, and within the validity limits of the undertaken approximations, an interesting connection can be used between extrinsic curvature properties of an hypersurface of a Euclidean space $\mathbb{R}^{N+1}$ and its Betti numbers (the diffeomorphism-invariant dimensions of the cohomology groups of the hypersurface, thus topological invariants) [38]. This connection is made by Pinkall's inequality given in the following.

Denoting by

$$\sigma(L_x)^2 = \frac{1}{N^2}\sum_{i<j}(\kappa_i - \kappa_j)^2$$

the dispersion of the principal curvatures of the hypersurface, then after Pinkall's theorem [39]

$$\frac{1}{\mathrm{vol}(\mathbb{S}^N)}\int_{\Sigma_v^N}[\sigma(L_x)]^N\ d\mu(x) \geq \sum_{i=1}^{N-1}\left(\frac{i}{N-i}\right)^{N/2-i}\ b_i(\Sigma_v^N)\ , \tag{30}$$

where $b_i(\Sigma_v^N)$ are the Betti numbers of the manifold Σ_v^N immersed in the Euclidean space $\mathbb{R}^{N+1}$, $\mathbb{S}^N$ is an N-dimensional sphere of unit radius, and $\mu(x)$ is the measure on Σ_v^N.

With the help of the Hölder inequality for integrals we have

$$\int_{\Sigma_v^N}[\sigma(L_x)]^2\ d\mu(x) \leq \left[\int_{\Sigma_v^N}\{[\sigma(L_x)]^2\}^{N/2}d\mu(x)\right]^{2/N}\left[\int_{\Sigma_v^N}d\mu(x)\right]^{1/(1-2/N)} \tag{31}$$

whence, at large N,

$$\left[\int_{\Sigma_v^N}d\mu(x)\right]^{-1}\int_{\Sigma_v^N}[\sigma(L_x)]^2\ d\mu(x) \leq \left[\int_{\Sigma_v^N}\{[\sigma(L_x)]^2\}^{N/2}d\mu(x)\right]^{2/N} \tag{32}$$

this inequality becomes an equality when $|f|^p/\|f\|_p^p = |g|^q/\|g\|_q^q$ almost everywhere [40], where $\|f\|_p$ is the standard L^p norm $\|f\|_p = \left(\int_S |f|^p d\mu(x)\right)^{1/p}$, where S is a measurable space. In the inequalities above $g(x) = 1$, thus the Hölder inequality becomes an equality when $|f|^p = \|f\|_p^p/\int_S d\mu(x)$, that is, when $|\sigma(L_x)|^N$ equals its average value almost everywhere on Σ_v^N. Introducing a positive remainder function $r(v)$, Eq.(32) is rewritten as

$$\left[\int_{\Sigma_v^N}d\mu(x)\right]^{-1}\int_{\Sigma_v^N}[\sigma(L_x)]^2\ d\mu(x) = \left[\int_{\Sigma_v^N}\{[\sigma(L_x)]^2\}^{N/2}d\mu(x)\right]^{2/N} - r(v)\ . \tag{33}$$

For the model under investigation, the pointwise dispersion of the principal curvatures of the potential level sets actually displays a limited variability from point to point. This follows from the observation that the numerically computed variance of the mean curvature in Eq.(23) is very fastly convergent to its asymptotic value, independently of the initial condition. The spread of the values of $\sigma_M = N\langle Var(M)\rangle_{\Delta t} = N[\langle M^2\rangle_{\Delta t} - \langle M\rangle_{\Delta t}^2]$, numerically computed along short segments of time duration $\Delta t = 100$, out of long phase space trajectories - of a time duration of $t = 10^6$ - typically amounts to $3-5\%$. As a consequence, on this slightly coarse-grained manifold the condition to make Hölder inequality an equality is not far from being satisfied, what indicates that in the case under study the Hölder inequality is reasonably tight and the remainder $r(v)$ can be considered as a small correction.

Then, using

$$\sigma_M = N[\langle M^2\rangle_{\Sigma_v} - \langle M\rangle^2_{\Sigma_v}] \sim \left[\int_{\Sigma_v^N} d\mu(x)\right]^{-1} \int_{\Sigma_v} [\sigma(L_x)]^2 \, d\mu(x) \tag{34}$$

together with Eq.(33) and the Pinkall inequality, one finally gets

$$\sigma_M \sim \left[\int_{\Sigma_v^N} \{[\sigma(L_x)]^2\}^{N/2} d\mu(x)\right]^{2/N} - r(v) \sim \left[\mathrm{vol}(\mathbb{S}^N) \sum_{i=1}^{N-1} \left(\frac{i}{N-i}\right)^{N/2-i} b_i(\Sigma_v^N)\right]^{2/N} - r(v) \ , \tag{35}$$

that is, the observable $\sigma_M(v)$ is explicitly related with the topology of the level sets Σ_v^N. This relation, even being an approximate one, is definitely non-trivial because there are very few possibilities of relating total curvature properties of a manifold with its topological invariants. On the other hand, both Pinkall's inequality and the Hölder inequality are sufficiently tight to make Eq.(35) meaningful. In fact, in addition to the already given arguments concerning the Hölder inequality in Eq.(32), Pinkall's inequality stems from the Morse inequalities $\mu_k(M) \geq b_k(M)$ which relate the Morse indexes $\mu_k(M)$ to the Betti numbers $b_k(M)$ of a manifold M (Pinkall's inequality would be replaced by an equality if written with Morse indexes), and these Morse inequalities are very tight since the alternating sums of Morse indexes and of Betti numbers, respectively, give the same result (the Euler characteristic). Therefore, the integral in the l.h.s. of Eq.(35) necessarily follows the topological variations of the Σ_v^N described by the weighted sum of its Betti numbers. The consequence is that a suitable variation with v of the weighted sum of the Betti numbers of a Σ_v^N can be *sufficient* to entail a sudden change of the convexity of the function $\sigma_M(v)$, as reported in Figure 9, and thus entail a discontinuity of its second derivative [41]. Sufficiency means that independently of $r(v)$, if some sharp change of the topology of the Σ_v^N takes place, then $\sigma_M(v)$ is affected.

On the other hand, the existence of a relationship between thermodynamics and configuration space topology is provided by the following exact formula [7, 19]

$$\begin{aligned} S_N^{(-)}(v) &= (k_B/N) \log \left[\int_{M_v^N} d^N q\right] \\ &= \frac{k_B}{N} \log \left[vol[M_v^N \setminus \bigcup_{i=1}^{\mathcal{N}(v)} \Gamma(x_c^{(i)})] \ + \sum_{i=0}^{N} w_i \ \mu_i(M_v^N) + \mathcal{R} \right] , \end{aligned} \tag{36}$$

where $S_N^{(-)}$ is the configurational entropy, and the $\mu_i(M_v^N)$ are the Morse indexes (in one-to-one correspondence with topology changes) of the submanifolds $\{M_v^N = V_N^{-1}((-\infty, v])\}_{v\in\mathbb{R}}$

of configuration space; in square brackets: the first term is the result of the excision of certain neighbourhoods of the critical points of the interaction potential from M_v^N; the second term is a weighed sum of the Morse indexes, and the third term is a smooth function of N and v. Again, sharp changes in the potential energy pattern of at least some of the $\mu_i(M_v^N)$ (thus of the way topology changes with v) affect $S_N^{(-)}(v)$ and its derivatives.

In other words, both the jump of the second derivative of the entropy and of the second derivative of σ_M are possibly rooted in the same topological ground, where some adequate variation of the topology of the Σ_v^N - foliating the configuration space - takes place. Notice that even if in Eq.(36) $S_N^{(-)}(v)$ depends on the topology of the M_v^N through the Morse indexes $\mu_i(M_v^N)$, in the framework of Morse theory a topology change of a level set Σ_v^N is always associated with a topology change of the associated manifold M_v^N of which Σ_v^N is the boundary [42].

Summarizing, the topology changes which seem to be indirectly detected by the function $\sigma_M(u)$ can affect the configurational entropy $S_N(v)$ and its tendency to develop an asymptotic discontinuity of $\partial_v^2 S_\infty(v)$ (we use u and v interchangeably). Notice that directly computing the Betti numbers of the Σ_v^N, or of the M_v^N, is in general undoable. In some very special cases [13, 14] it has been possible to analytically compute the Morse indexes of these manifolds, which are good estimators of the Betti numbers. But in general one has to necessarily resort to known results in differential topology relating total curvature properties of a manifold with its topological invariants. This is the case of the Gauss-Bonnet-Hopf theorem for hypersurfaces of N-dimensional Euclidean spaces, where the integral of the Gauss-Kronecker curvature is proportional to the Euler characteristic of the hypersurface, of the Chern-Lashof theorem where the integral of the modulus of the Gauss-Kronecker curvature gives the sum of the Morse indexes of the manifold, or the Pinkall theorem which has been used in the present work. And, in general, we can wonder how to combine Ehrenfest's classification of phase transitions in the microcanonical configuration space, put forward in Section III.C, with the topological transitions in the absence of an order parameter, for instance, we can wonder how the present analysis of a first order transition without symmetry breaking would work in the case of second order transitions without symmetry breaking. In this case, Eqs. (36) and (37) qualitatively indicate that suitable variations with v of the $\{\mu_i(M_v^N)\}$, or with E of the $\{b_i(\Sigma_E^N)\}$, can entail singular behaviors of any desired derivative of the entropy. For a second order transition a discontinuity of the third derivative of the entropy is required, but, again, this can be related to topology only through some theorem of differential topology, thus through the energy variation of total geometric quantities.

Finally, in Appendix we give a more technical account of how the non-trivial contribution to the homology groups of the energy level sets Σ_E^N comes from the homology groups of the configuration space submanifolds $M_v^N \subset M_E^N$ and $\Sigma_v^N \subset \Sigma_E^N$. Therefore, the topology variations of the Σ_v^N imply topology variations of the Σ_E^N, and these necessarily affect also the functional dependence on E of the total entropy $S_N(E)$. In fact, the variation with v of the topology of the Σ_v^N is in one-to-one correspondence with some variation with v of the Betti numbers $b_i(\Sigma_v^N)$ entering Eq.(35), and this entails the variation with E of the Betti numbers $b_i(\Sigma_E^N)$, so that, according to the following formula [7] for the total entropy

$$S_N(E) \approx \frac{k_{\rm B}}{N} \log \left[{\rm vol}(\mathbb{S}_1^{N-1}) \sum_{i=0}^{N} b_i(\Sigma_E^N) + \mathcal{R}_1(E) \right] + \mathcal{R}_2(E) \ , \tag{37}$$

where $\mathcal{R}_1(E)$, and $\mathcal{R}_2(E)$ are smooth functions, we see that the variation with v of the topology of the Σ_v^N implies also the variation with E of the total entropy.

IV. CONCLUDING REMARKS

We have tackled the problem of characterizing a phase transition in the absence of global symmetry breaking from the point of view of Hamiltonian dynamics and related geometrical and topological aspects. In this condition the Landau classification of phase transitions does not apply, because no order parameter - commonly associated with a global symmetry - exists. The system chosen is inspired by the dual of the Ising model, and the discrete variables are replaced by continuous ones. We stress that our work has nothing to do with the true dual Ising model, which has just suggested how to define a classical Hamiltonian system with a local (gauge) symmetry. Since the ergodic invariant measure for generically non-integrable Hamiltonian systems is the microcanonical measure in phase space, studying phase transitions through Hamiltonian dynamics is the same as studying them in the microcanonical ensemble.

A standard analysis has been performed to locate the phase transition and to determine its order through the shape of the caloric curve, $T = T(E)$, which appeared typical of a first order phase transition. The presence of energy intervals of negative specific heat are indicative of ensemble nonequivalence. At variance with what has been systematically observed for systems undergoing symmetry-breaking phase transitions, the energy pattern of the largest Lyapunov exponent does not allow to locate the transition point.

After the Yang-Lee theory, phase transitions are commonly associated with a loss of analyticity of a thermodynamic potential entailing non-analytic patterns of thermodynamic observables (the pertinent potential depends on the statistical ensemble chosen). However, there is no evidence of the existence of genuinely non-analytic energy pattern of some observable for our gauge model, in fact, no bifurcating order parameter exists, the caloric curve is a regular function, and the peaks of the specific heat are just due to horizontal tangencies to the caloric curve and a-priori are not necessarily due to singularities of the entropy. Nevertheless, an analyticity loss of the entropy has been directly detected through a point of discontinuity of the second derivative of the entropy (or at least a finite size version of such a discontinuity), thus an asymptotic divergence of its third derivative. As a consequence, this fits properly into the classification scheme *à la* Ehrenfest discussed in Section III.C for the microcanonical ensemble. Then, by resorting to the classification of microcanonical phase transitions based on inflection-point analysis of Ref.[35] we have been able to interestingly complement the interpretation of our numerical outcomes for the thermodynamic observables.

Remarkably, we have found a quantity, $\sigma_M(v)$, that - by measuring the total degree of inhomogeneity of the extrinsic curvature of the potential level sets $\Sigma_v = V^{-1}(v)$ in configuration space - identifies the phase transition point. This quantity is not a thermodynamic observable, has a purely geometric meaning, and displays a discontinuity of its second derivative in coincidence with the same kind of discontinuity displayed by the entropy. Rather than being a trivial consequence of the presence of the phase transition, the peculiar change of the geometry of the $\{\Sigma_v^N\}_{v\in\mathbb{R}}$ so detected is the deep cause of the singularity of the entropy. In fact, the potential level sets are simply subsets of $\mathbb{R}^N$ defined as $\Sigma_v^N = \{(q_1,\dots,q_N)\in\mathbb{R}^N | V(q_1,\dots,q_N) = v\}$, whose ensemble $\{\Sigma_v^N\}_{v\in\mathbb{R}}$ foliates the configuration space; the volume $\Omega(v,N)$ - of each leaf Σ_v^N - and the way it varies as a function of v is just a matter of geometrical/topological properties of the leaves of the foliation. These properties entail the v-dependence of the entropy $S_N(v) = (1/N)\log\Omega(v,N)$, and, of course, its differentiability class. This is why the v-pattern of the quantity $\sigma_M(v)$ is not the consequence of the presence of a phase transition but, rather, the reason of its appearance. This is already a highly non trivial fact indicating that whether a physical system can undergo a phase transition is somehow already encoded in the interactions among its degrees of freedom described by the potential function $V(q_1, \dots, q_N)$, independently of the statistical ensemble chosen to describe its macroscopic observables. However, we can wonder if one can go deeper by looking for the origin of the peculiar changes with v of the geometry of the Σ_v^N. Actually, by resorting to a theorem in differential topology, and with some approximations, these geometrical changes are strongly suggestive of the presence of changes of the topology of both the potential level sets in configuration space and the energy level sets in phase space. Therefore, although one single example cannot be taken as a rule, and certainly much work remains to be done, the results of the present work go in the direction of supporting the topological theory of phase transitions.

Moreover, since the practical computation of $\sigma_M(v)$, or of $\sigma_M(E)$, is rather straightforward, this can be used to complement the study of transitional phenomena in the absence of symmetry-breaking, as is the case of: liquid-gas change of state, Kosterlitz-Thouless transitions, glasses and supercooled liquids, amorphous and disordered systems, folding transitions in homopolymers and proteins, both classical and quantum transitions in small N systems. With respect to the latter case, a remark about the geometrical/topological theory is in order. In nature, phase transitions (that is major qualitative physical changes) occur also in very small systems with N much smaller than the Avogadro number, but their mathematical description through the loss of analyticity of thermodynamic observables requires the asymptotic limit $N \to \infty$. To the contrary, within the geometrical/topological framework a sharp difference between the presence or the absence of a phase transition can be made also at any finite and even very small N. At finite N, the microscopic states that significantly contribute to the statistical averages of thermodynamic observables are spread in regions of configuration space which get narrower as N increases, so that the statistical measures better concentrate on a specific potential level set thus better detecting its sudden and major geometry and topology changes, if any. Eventually, in the $N \to \infty$ limit the extreme sharpening of the effective support of the measure leads to a geometry-induced, and possibly also a topology-induced, nonanalyticity of thermodynamic observables [7].

Furthermore, even if somewhat abstract, the model studied in the present work has the basic properties of a lattice gauge model, that is, its potential depends on the circulations of the gauge field on the plaquettes, so that the geometrical/topological approach developed here could be also of some interest to the numerical investigation of phase transitions of

Euclidean gauge theories on lattice. In fact, computing $\sigma_M(v)$, or $\sigma_M(E)$, is definitely much easier than computing the Wilson loop, commonly adopted in place of an order parameter for gauge theories. Actually, a few decades ago, several papers on the microcanonical formulation of quantum field theories appeared [43, 44], motivated by the fact that in statistical mechanics and in field theory there are systems for which the canonical description is pathological, but the microcanonical is not, also arguing, for instance and among other things, that a microcanonical formulation of quantum gravity may be less pathological than the usual canonical formulation [45–48]. More recent works can also be found on these topics [49–52]. Moreover, in quantum many-body systems at zero temperature quantum phase transitions can occur by varying some parameter of the Hamiltonian of the system. The different phases correspond to qualitatively different quantum states which are not characterized by an order parameter [53, 54] but rather described by suitably defined topological order. These topological phase transitions, occurring in the absence of symmetry breaking, are investigated by resorting to the methods of quantum field theory [55]. Among the other topics, attention has been given to the possible existence of second order phase transitions in the absence of symmetry breaking, thus in the absence of an order parameter. Such a possibility, just to give an example, has been suggested for the case of the deconfining transition of $SU(N)$ gauge theories in 2+1 dimensions for $N \leq 3$ [56]. It is worth mentioning that, in principle, the topological approach to classical phase transitions - addressed in the present work - and the just mentioned topological treatment of quantum transitions could be linked by Wick's analytic prolongation to imaginary times of the path-integral generating functional of quantum field theory, this allows to map a quantum system onto a formally classical one described by a classical partition function written with the euclidean Lagrangian action, on lattice to have a countable number of degrees of freedom [7].

Finally, as a side issue, it is provided here an example of statistical ensemble non-equivalence in a system with short-range interactions. Ensemble non-equivalence is another topic which is being given much attention in recent literature [57].

APPENDIX

A. Relation between topological changes of the Σ_v and of the Σ_E

Now, let us see why a topological change of the configuration space submanifolds $\Sigma_v = V^{-1}(v)$ (potential level sets) implies the same phenomenon for the Σ_E. The potential level sets are the basic objects, foliating configuration space, that represent the nontrivial topological part of phase space. The link of these geometric objects with microcanonical entropy is given by

$$S^{(-)}(E) = \frac{k_B}{2N} \log \int_0^E d\eta \int d^N p\ \delta(\sum_{\mathbf{i}} p_{\mathbf{i}}^2/2 - \eta) \int_{\Sigma_{E-\eta}} \frac{d\sigma}{\|\nabla V\|}\ . \tag{38}$$

As N increases the microscopic configurations giving a relevant contribution to the entropy, and to any microcanonical average, concentrate closer and closer on the level set $\Sigma_{\langle E-\eta \rangle}$. A link among the topology of the energy level sets and the topology of configuration space can be established for systems described by a Hamiltonian of the form $\mathcal{H}_N(p,q) = \sum_{i=1}^N p_i^2/2 + V_N(q_1, ..., q_N)$.

In fact, (using a cumbersome notation for the sake of clarity) the level sets $\Sigma_E^{\mathcal{H}_N}$ of the energy function $\mathcal{H}_N$ can be given by the disjoint union of a trivial unitary sphere bundle (representing the phase space region where the kinetic energy does not vanish) and the hypersurface in configuration space where the potential energy takes the total energy value (details are given in [58])

$$\Sigma_E^{\mathcal{H}_N} \text{ homeomorphic to } M_E^{V_N} \times \mathbb{S}^{N-1} \bigsqcup \Sigma_E^{V_N} \tag{39}$$

where $\mathbb{S}^n$ is the n-dimensional unitary sphere and

$$M_c^f = \{x \in \mathrm{Dom}(f) | f(x) < c\}\,,$$
$$\Sigma_c^f = \{x \in \mathrm{Dom}(f) | f(x) = c\}\,. \tag{40}$$

The idea that finite N topology, and "asymptotic topology" as well, of $\Sigma_E^{\mathcal{H}_N}$ is affected by the topology of the accessible region of configuration space is suggested by the *Künneth formula*: if $H_k(X)$ is the k-th homological group of the topological space X on the field $\mathbb{F}$ then

$$H_k(X \times Y; \mathbb{F}) \simeq \bigoplus_{i+j=k} H_i(X;\mathbb{F})\ \otimes\ H_j(Y;\mathbb{F})\ . \tag{41}$$

Moreover, as $H_k\left(\sqcup_{i=1}^N X_i, \mathbb{F}\right) = \bigoplus_i^N H_k(X_i, \mathbb{F})$, it follows that:

$$
\begin{aligned}
& H_k\left(\Sigma_E^{\mathcal{H}_N}, \mathbb{R}\right) \\
& \simeq \bigoplus_{i+j=k} H_i\left(M_E^{V_N}; \mathbb{R}\right) \otimes\ H_j\left(\mathbb{S}^{N-1}; \mathbb{R}\right) \oplus H_k\left(\Sigma_E^{V_N}; \mathbb{R}\right) \\
& \simeq H_{k-(N-1)}\left(M_E^{V_N}; \mathbb{R}\right) \otimes \mathbb{R} \oplus H_k\left(M_E^{V_N}; \mathbb{R}\right) \otimes \mathbb{R} \\
& \oplus H_k\left(\Sigma_E^{V_N}; \mathbb{R}\right)
\end{aligned}
\tag{42}
$$

the r.h.s. of Eq.(42) shows that the topological changes of $\Sigma_E^{\mathcal{H}_N}$ only stem from the topological changes in configuration space.

ACKNOWLEDGMENTS

The authors acknowledge the financial support of the Future and Emerging Technologies (FET) Program within the Seventh Framework Program (FP7) for Research of the European Commission, under the FET-Proactive TOPDRIM Grant No. FP7-ICT-318121. The project leading to this publication has received funding also from the Excellence Initiative of Aix-Marseille University - A*Midex, a French "Investissements d'Avenir" programme. Roberto Franzosi thanks the support by the QuantERA projects Q-Clocks. Cecilia Clementi acknowledges support by the National Science Foundation (CHE-1265929, CHE-1738990, and PHY-1427654), the Welch Foundation (C-1570), and the Einstein Foundation in Berlin.

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