Models with Phase Transition Triggered by Double-Well Potentials and Dumbbell Equipotential Hypersurfaces

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(Dated: April 1, 2019)

In some recent papers some theorems on sufficient conditions for the occurrence of \( \mathbb{Z}_2 \)-symmetry breaking phase transition (SBPT) have been showed making use of geometric-topological features of the potential energy landscape. In particular \( \mathbb{Z}_2 \)-SBPT can be triggered by double-well potentials and dumbbell-shaped equipotential hypersurfaces. In this paper we introduce some models with \( \mathbb{Z}_2 \)-SBPT, that, due to their essential feature, show in the clearest way the generating-mechanism of \( \mathbb{Z}_2 \)-SBPTs above-mentioned. These models, despite they are not physical models, may enlighten some aspects of phase transitions again remained obscure. For instance, the study of the relation with the critical points, and the topology of the equipotential hypersurfaces can be greatly simplified by the fact that the potentials have only three critical points. A comparison with the mean-field \( \phi^4 \) model has been made revealing the same geometric picture of the models introduced in this paper.

PACS numbers: 75.10.Hk, 02.40.-k, 05.70.Fh, 64.60.Cn
Keywords: Phase transitions; potential energy landscape; configuration space; symmetry breaking

I. INTRODUCTION

Phase transition are very common in nature. They are sudden changes of the macroscopic behaviour of a natural system composed by many interacting parts occurring while an external parameter is smoothly varied. Phase transitions are an example of emergent behaviour, i.e. of a collective properties having no direct counterpart in the dynamics or structure of individual atoms \[34\]. The successful description of phase transitions starting from the properties of the interactions between the components of the system is one of the major achievements of equilibrium statistical mechanics.

From a statistical-mechanical point of view, describing a system at constant temperature \( T \), a phase transition occurs at special values of the temperature called transition points, where thermodynamic quantities such as pressure, magnetization, or heat capacity, are non-analytic functions of \( T \); these points are the boundaries between different phases of the system. Phase transitions are strictly related to the phenomenon of spontaneous symmetry breaking. For example, below the Curie temperature in a natural magnet the \( O(3) \) symmetry is spontaneous broken because of the occurrence of a spontaneous magnetization. In this paper we mostly consider the origin of this aspect, and secondarily the origin of the non-analyticities in the thermodynamic functions.

Despite great achievements in our understanding of phase transitions, yet, the situation is not completely satisfactory. For example, while necessary conditions for the presence of a phase transitions can be found, nothing general is known about sufficient conditions, apart some particular cases \[6\]; no general procedure is at hand to tell if a system where a phase transition is not ruled out from the beginning does have or not such a transition without computing the partition function \( Z \). This might indicate that our deep understanding of this phenomenon is still incomplete.

These considerations motivate a study of the deep nature of phase transitions which may also be based on alternative approaches. One of them is the geometric-topological approach based on the study of the landscape of the energy potential. In particular the equipotential hypersurfaces, i.e. the \( v \)-level sets, gain a great importance inside this approach. This idea has been discussed and tested in many recent papers \[2, 5, 6, 10, 12, 23, 24, \]

In particular, in the paper \[3\] it has been shown a theorem which links the occurrence of a \( \mathbb{Z}_2 \)-SBPT to dumbbell-shaped \( v \)-level sets of the potential. Intuitively, a set is said dumbbell-shaped when it shows two major components connected by a shrink neck. Something like this SBPT generating-mechanism has been put forward also in the recent papers \[21, 22\]. According to the theorem, a spontaneous \( \mathbb{Z}_2 \)-SB is entailed by dumbbell-shaped \( v \)-level sets of the potential, and the critical potential \( v_c \) is in correspondence of a critical \( v_c \)-level set in the sense that it is the boundary between the set of the dumbbell \( v \)-level sets at \( v < v_c \) and the set of the non-dumbbell ones at \( v > v_c \). A great advantage with respect to the traditional definition of phase transitions is that here the definition holds for finite \( N \) without resorting to the thermodynamic limit. Since in the last decades many examples of transitional phenomena in systems far from the thermodynamic limit have been found (e.g. in nuclei, atomic clusters, biopolymers, superconductivity, superfluidity), a description of phase transition valid also for finite systems would be desirable.

In this paper we introduce some models showing \( \mathbb{Z}_2 \)-SBPT which illustrate in the clearest way the generating-mechanism based on the concept of dumbbell-shaped \( v \)-
level sets generated in turn by double-well potentials. The models do not describe any physical system, so that their usefulness is for giving hints about physical models, and for didactic purposes. In Sec. II we present the framework of the geometric approach to SBPTs in the canonical treatment. In Sec. III we build a model with non-smooth potential. In Sec. IV we derive from the model of Sec. III a model with smooth potential. In V we introduce another model with smooth potential written as an explicit function of coordinates. The landscape of the models with smooth potential is characterized by the fact that they have three critical points only. Finally, in Sec. VI we revisit the well known mean-field model of Sec. III a model with smooth potential. In VI we assume the potential to be lower bounded.

Hereafter we will refer to the canonical treatment, although the dumbbell-shaped \( v \)-level set approach can be extended to the microcanonical one. Consider an \( N \) degrees of freedom system with Hamiltonian given by

\[
H(p, q) = T + V = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(q). \tag{1}
\]

Let \( M \subseteq \mathbb{R}^N \) be the configuration space. The partition function is by definition

\[
Z(\beta, N) = \int_{\mathbb{R}^N \times M} dp dq e^{-\beta H(p, q)} = \int_{\mathbb{R}^N} dp \int_{M} dq e^{-\beta V(q)} = Z_{\text{kin}} Z_{c} \tag{2}
\]

where \( \beta = \frac{1}{T} \) (in unit \( k_B = 1 \)), \( Z_{\text{kin}} \) is the kinetic part of \( Z \), and \( Z_{c} \) is the configurational part. In order to develop what follows we assume the potential to be lower bounded. \( Z_{c} \) can be written as follows

\[
Z_{c} = N \int_{v_{\min}}^{+\infty} dv e^{-\beta N v} \int_{\Sigma_{v,N}} \frac{d\Sigma}{\sqrt{\nabla V}} \tag{3}
\]

where \( v = \frac{V}{N} \) is the potential per degree of freedom, and the \( \Sigma_{v,N} \)'s are the \( v \)-level sets defined as

\[
\Sigma_{v,N} = \{ q \in M : v(q) = v \}. \tag{4}
\]

The \( \Sigma_{v,N} \)'s are the boundaries of the \( M_{v,N} \)'s (\( \Sigma_{v,N} = \partial M_{v,N} \)) defined as

\[
M_{v,N} = \{ q \in M : v(q) \leq v \}. \tag{5}
\]

The set of the \( \Sigma_{v,N} \)'s is a foliation of configuration space \( M \) while varying \( v \) between \( v_{\min} \) and \( +\infty \). The \( \Sigma_{v,N} \)'s are very important submanifolds of \( M \) because as \( N \to \infty \) the canonical statistic measure shrinks around \( \Sigma_{\bar{v}(T),N} \), where \( \bar{v}(T) \) is the average potential per degree of freedom. Thus, \( \Sigma_{\bar{v}(T),N} \) becomes the most probably accessible \( v \)-level set by the representative point of the system.

This fact may have significant consequences on the symmetries of the system because of the fact that the ergodicity may be broken in the thermodynamic limit by the mechanism showed in [3].

We can make the same considerations for \( Z_{\text{kin}} \), but the related submanifolds \( \Sigma_{t,N} \), where \( t = \frac{1}{T} \) is the kinetic energy per degree of freedom, are all trivially bounded, thus they cannot affect the symmetry properties of the system. Furthermore, \( Z_{\text{kin}} \) is analytic at any \( T \) in the thermodynamic limit, so that it cannot entail any loss of analyticity in \( Z \).

For the above considerations, hereafter we will consider only the configurational part of \( Z \), so as for the thermodynamic functions.

III. MODEL OF REVOLUTION

In [6] it has been given a sufficiency condition for the occurrence of a \( Z_2 \)-SBPT. This states that the potential landscape has two absolute minima separated by a gap proportional to \( N \). Here our purpose is to follow this path, thus to build a \( Z_2 \)-symmetric double-well potential in \( N \)-dimensions with the gap between the wells proportional to \( N \).

Let \( q_1, \ldots, q_N \) be the standard coordinate system of \( \mathbb{R}^N \). The starting point is to set a new coordinate system

\[
\tilde{m}, \tilde{q}_1, \ldots, \tilde{q}_{N-1}, \tag{6}
\]

where the direction of the first coordinate \( \tilde{m} = \sqrt{N} m \) is the axis orthogonal to the hyperplane \( \sum_{i=1}^{N} q_i = 0 \) passing by the origin, \( m \) is nothing but the magnetization \( m = \frac{1}{N} \sum_{i=1}^{N} q_i \), and \( \tilde{q}_1, \ldots, \tilde{q}_{N-1} \) are orthonormal coordinate system orthogonal to \( \tilde{m} \).

Define the potential as a function of \( m \)

\[
V = N (-Jm^2 + m^4), \tag{7}
\]

where \( J > 0 \) plays the role of the coupling constant. \( V \) is flat in any direction orthogonal to \( \tilde{m} \). \( V \) has two degenerate absolute minima at \( m = \pm \sqrt{\frac{J}{2}} \) of value \( -\frac{1}{4} N J^2 \), whose coordinates in the coordinate system [6] are \( (\pm \sqrt{\frac{N J}{2}}, \tilde{q}_1, \ldots, \tilde{q}_{N-1}) \) for any \( \tilde{q}_i \), \( i = 1, \ldots, N - 1 \).

Further, \( V \) has a degenerate relative maximum at \( m = 0 \) of coordinates \( (0, \tilde{q}_1, \ldots, \tilde{q}_{N-1}) \) for any \( \tilde{q}_i \).

The \( V \)-level sets of \( V \) describe hyperplanes at constant magnetization of \( \mathbb{R}^N \), that for convenience we define in the standard coordinate system as follows

\[
\pi_{m,N} = \{ q \in \mathbb{R}^N : \frac{1}{N} \sum_{i=1}^{N} q_i = m \}. \tag{8}
\]
or in the coordinate system

\[ \pi_{m,N} = \{(\bar{m}, \bar{q}_1, \ldots, \bar{q}_{N-1}) \in \mathbb{R}^N : \bar{m} = \sqrt{N} m\}. \tag{9} \]

Define the configuration space of the system \( M \subseteq \mathbb{R}^N \). If we assumed \( M = \mathbb{R}^N \), the magnetization would be frozen at \( \pm \sqrt{\frac{2}{N}} \) for any value of \( T \), because \( V \) is not a double-well potential due to its flatness in the directions orthogonal to \( \bar{m} \). In order to create the double-well, we add a constraint on \( M \) in such a way that the Taylor expansion of the entropy at fixed \( m \)

\[ s_N(m) = \frac{1}{N} \ln \text{vol}(M \cap \pi_{m,N}) \tag{10} \]

has a non-vanishing second-order term. This term will compete with the second-order term of \( V \) giving rise to the critical temperature \( T_c \). To attain this effect, the simplest choice is

\[ \text{vol}(M \cap \pi_{m,N}) = e^{-(N-1)m^2} \tag{11} \]

which yields in the thermodynamic limit

\[ s(m) = \lim_{N \to \infty} s_N(m) = -m^2. \tag{12} \]

Now, the problem is how to fit up these volumes to complete the definition of configuration space \( M \). We can give them the shape of an \((N-1)\)-ball contained in the hyperplane \( \pi_{m,N} \) with the center belonging to the line orthogonal to \( \pi_{m,N} \) and passing through the origin. The radius of the \((N-1)\)-ball is chosen in such a way to yield the volume \((11)\). So built, the configuration space \( M \) has a shape of an infinite \( N \)-dimensional 'spindle'. The potential, besides the \( \mathbb{Z}_2 \) symmetry, has also an \( O(N-1) \) one with respect to the line orthogonal to the \( \pi_{m,N} \)'s and passing through the origin (from which the name model of revolution).

The free energy results to be

\[ f = v(m) - Ts(m) = (T - J)m^2 + m^4, \tag{13} \]

where \( v = \frac{\partial f}{\partial m} \). \( T_c = J \) is the critical temperature of the system. The spontaneous magnetization is given by a minimization process of \( f \) with respect to \( m \), and results as follows

\[ \langle m \rangle = \begin{cases} \pm \sqrt{2}(J - T)^{\frac{1}{2}} & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c. \end{cases} \tag{14} \]

The free energy as a function of \( T \), the average potential, and the specific heat are, respectively,

\[ f(m(T),T) = \begin{cases} -\frac{1}{4}(J-T)^2 & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c. \end{cases} \tag{15} \]

\[ \langle v \rangle = -T^2 \frac{\partial}{\partial T} \left( \frac{f}{T} \right) = \begin{cases} -\frac{1}{4}(JT^2) & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c. \end{cases} \tag{16} \]

FIG. 1: Model of Sec. III for \( J = 1 \). From top to bottom and from left to right: magnetization, free energy, average potential, and specific heat as functions of the temperature. The blue graphs are at \( N = 10, 100, \) and \( 1000 \), while the red ones are at \( N = \infty \).

\[ c_v = \frac{\partial}{\partial T} \left( \frac{f}{T} \right) = \begin{cases} \frac{T}{2} & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c. \end{cases} \tag{17} \]

The partition function is

\[ Z_N = \sqrt{N} \int dm e^{-N(-m^2 + m^4)} \tag{18} \]

which permits the calculation at finite \( N \) of the thermodynamic functions (see Fig. 1). The uniform convergence toward the \( N \to \infty \) limit is broken in correspondence of the critical temperature \( T_c \).

A. On the origin of phase transitions

In a great effort has been put in trying to understand the deep origin of a phase transition (PT) meant as a loss of analyticity in the thermodynamic functions. The leading idea is the topological hypothesis, according to which a phase transition is entailed by some suitable topological changes in the equipotential hyper surface, i.e. the \( v \)-level sets. Here, our purpose is not to validate or not the topological hypothesis, but make some trivial considerations about that question.

The free energy \( f \) in the \((m,T)\)-plane in the thermodynamic limit is an analytic function, but, e.g. this is not the case of the spontaneous magnetization as a function of \( T \). By resorting to the Dini theorem (or implicit function theorem) we know that the graph of the zeroes of the partial derivative with respect to \( m \) of \( f \), i.e. the spontaneous magnetization, is an analytic function too. More precisely, if \( f(m,T) \in C^k \), then also \( m(T) \in C^k \) for \( k = 1, \ldots, \infty \).

The singular point in the graph of \( m(T) \) arises because it is the union of two analytic branches of \( m(T) \) that cannot be jointed without passing through a non-analytic
algebraic manipulations, we obtain
\[ \langle H \rangle = \frac{1}{2} H^\pm, \]  
from which we get \( \delta = 3 \). To find out \( \gamma \) we solve
\[ \frac{\partial^2 f}{\partial m \partial H} = -1 + 2(T - J) \frac{\partial f}{\partial m} + 12m^2 \frac{\partial f}{\partial m} = 0, \]  
from which we get the magnetic susceptibility
\[ \chi(T) = \frac{\partial f}{\partial m} = \frac{1}{2(T - J) - 12m^2}, \]  
where, by inserting \( m(T) \) given in (14), we obtain
\[ \chi(T) = \begin{cases} \frac{1}{2(T - J)} & \text{if } T \leq T_c, \\ \frac{1}{10(T - J)} & \text{if } T \geq T_c, \end{cases} \]  
from which \( \gamma = 1 \).

To conclude, the critical exponents are that of a classical second-order SBPT.

C. Other critical exponents and universality classes

We can generalize the definition of the potential (7) as follows
\[ V = N \left( -J|m|^k + |m|^l \right), \]  
with \( k, l \) naturals and \( 0 < k < l \). In order to give rise to the critical temperature, the volume of the subsets of configuration space \( M \) at constant \( m \) is generalized as \( e^{-(N-1)|m|^k} \).

For suitable choices of \( k, l \) the model of revolution belongs also to further universality classes than the classical one. For example, we will calculate the critical exponents for \( k = 8 \) and \( l = 16 \), which correspond to the universality class of the short-range 2D Ising model. The free energy in the thermodynamic limit is
\[ f = (T - J)m^8 + m^{16}, \]  
and the critical temperature is \( T_c = J \). By solving \( \frac{\partial f}{\partial m} = 0 \) we obtain the spontaneous magnetization
\[ \langle m \rangle = \begin{cases} \pm \frac{1}{2} (J - T)^\pm & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c, \end{cases} \]  
where \( T_c = J \), whence \( \beta = \frac{1}{2} \). \( \langle v \rangle (T) \) and \( c_v(T) \) are the same of the model of the previous Section, so that \( \alpha = 0 \).

After inserting the external magnetic field \( H \), the free energy becomes
\[ f = -mH + (T - J)m^8 + m^{16}, \]  
from which, by following the same procedure of the previous Section, we get
\[ \langle m \rangle (H) \propto H^{1/2}, \]  
whence \( \delta = 15 \), and
\[ \chi(T) \propto |T_c - T|^{-\gamma}, \]  
whence \( \gamma = \frac{7}{4} \), as promised.
where \( \nu = 0 \), and \( \nu_{min} = -\frac{1}{2} \). The \( \Sigma_{\nu,N} \)'s, i.e. the boundary of the \( M_{\nu,N} \)'s, do not include the curved lines. Bottom row: the same of top for \( H = 0.2 \); the \( \mathbb{Z}_2 \) symmetry is broken.

### D. Geometry and topology of the \( \nu \)-level sets and their link with the SBPT

In [6] a new way of understanding \( \mathbb{Z}_2 \)-SBPT has been introduced. It is based on the concept of dumbbell-shaped \( \nu \)-level sets which are defined in the following way. Any \( \nu \)-level set is in correspondence with the microcanonical density of states

\[
\omega_N(v, m) = \mu(\Sigma_{\nu,N} \cap \pi_{m,N}) = \int_{\Sigma_{\nu,N} \cap \pi_{m,N}} \frac{d\Sigma}{\|\nabla V\|},
\]

where \( m \) is the magnetization. A \( \nu \)-level set is called dumbbell-shaped if the function

\[
a_N(v, m) = \omega_N(v, m)^{\frac{1}{4}}
\]

does not take the maximum at \( m = 0 \). Note that this definition is valid for any \( N \), so that the study of phase transitions based on this framework is suitable non only in the thermodynamic limit, but also in the case when \( N \) is far from the thermodynamic limit.

The main result of this approach is a straightforward theorem which states that the \( \mathbb{Z}_2 \) symmetry is broken if, and only if, the \( \langle v \rangle (T) \)-level set corresponding to the temperature \( T \) is dumbbell-shaped for any \( N > N_0 \), where \( N_0 \) is a fixed natural. Furthermore, the critical average potential \( \nu_c = \langle v \rangle (T_c) \) is exactly in correspondence with the \( \nu \)-level set which is the boundary between the dumbbell-shaped levels and the non-dumbbell-shaped ones.

In [6] it has been given another topological sufficient condition (theorem 1 in the paper) for \( \mathbb{Z}_2 \)-SBPT which is a particular case of the hypotheses of the above-mentioned theorem. Simplifying the scenario, theorem 1 states that if the \( \Sigma_{\nu,N} \)'s are made by two disjointed components which are the image of each other under reflection of coordinates with respect the hyperplane \( \pi_{0,N} \) for \( v \in [v', v''] \), then the \( \mathbb{Z}_2 \) symmetry is broken for the same values of \( v \) provided that the last are accessible to the representative point of the system. If the \( \Sigma_{\nu,N} \)'s satisfy this hypothesis, it is immediate to verify that they are also dumbbell-shaped, whence the conclusion.

To find out the spontaneous magnetization we choose the values of \( m \) at which the function \( a(v,m) = \lim_{N \to \infty} a_N(v,m) \), or \( a_N(v,m) \) itself if we consider the case at finite \( N \), takes the maximum. \( a_N \) is linked to the microcanonical entropy \( s_N \) by the relation \( s_N = \ln a_N \). The so chosen value of \( m \) will be the spontaneous magnetization \( \langle m \rangle \) as a function of \( v \), which, in turn, is a function of \( T \): \( v = \langle v \rangle (T) \); whence \( \langle m \rangle (T) \). This definition is given for finite \( N \), but it can be directly extended to the thermodynamic limit provided that the limit exists.

After this brief introduction, let us consider the \( \nu \)-level sets of our model given by

\[
\Sigma_{\nu,N} = \{ q \in M : -J m^2 + m^4 = v \},
\]

Besides \( \Sigma_{\nu,N} \), it is convenient to define also the part of configuration space \( M \) below \( v \) as

\[
M_{\nu,N} = \{ q \in M : -J m^2 + m^4 \leq v \},
\]

which is nothing but the interior part of \( \Sigma_{\nu,N} : \partial M_{\nu,N} = \Sigma_{\nu,N} \).

Since

\[
m(v) = \pm \left( \frac{J \pm \sqrt{J + 4v}}{2} \right)^{\frac{1}{2}},
\]

we can distinguish three cases:

(i) \(-\frac{J}{4} \leq v < 0\); the equation above has four distinct solutions each of them corresponds to a single connected component of \( \Sigma_{\nu,N} \) made by an \( (N-1) \)-ball of volume \( e^{-(N-1)m(v)^2} \). These \( \Sigma_{\nu,N} \)'s satisfy the hypotheses of theorem 1 in [6] which implies \( \mathbb{Z}_2 \)-SB for the values of \( T \) such that \( \langle v \rangle (T) \in [-\frac{J}{4}, 0] \). Indeed, any connected component of any \( \Sigma_{\nu,N} \) is not the image of itself under the \( \mathbb{Z}_2 \) symmetry, as requested by the hypotheses of the theorem above-mentioned.

(ii) \( v = 0 \); equation (35) has three distinct solutions of which one equals zero. The connected components of \( \Sigma_{0,N} \) are three \( (N-1) \)-balls. In this case the \( \mathbb{Z}_2 \) symmetry is intact because the \( (N-1) \)-ball located at \( m = 0 \) has a greater volume than the other two.

(iii) \( v > 0 \); equation (35) has only two distinct solutions. According to theorem 1 in [6] the \( \mathbb{Z}_2 \) symmetry should be broken, but the values of \( v \) above zero are not accessible to the representative point of the system, so that the \( \Sigma_{0,N} \) plays the role of critical \( \nu \)-level set which separates the broken symmetry phase from the unbroken one.

For our model, we can express \( \nabla V \) in the coordinate system

\[
\nabla V = \left( \frac{\partial V}{\partial m}, 0, \cdots, 0 \right) = \left( \sqrt{N}(m^3 - 2m), 0, \cdots, 0 \right),
\]

(36)
whence \(|\nabla V|^{-1} = \left(\sqrt{N}|m^3 - 2m|\right)^{-1}\). The last quantity is constant onto any \(\pi_{m,N}\), so that it can be factorized in the integral \([31]\). In the limit \(N \to \infty\) the contribution of \(|\nabla V|^{-1}\) to \(\mu_{\Sigma}\) is 1, except at \(m = 0, \pm \frac{\sqrt{2}}{2}\) where it becomes infinite, hence we can substitute the measure \(\mu\) by the simpler standard volume \(e^{-(N-1)m^2}\) defined in \([11]\). The singularities at \(m = 0, \pm \frac{\sqrt{2}}{2}\) do not cause any uncertainty in locating the spontaneous magnetization because of the structure of the \(\Sigma_{v,N}\)’s for \(v = -\frac{1}{4}\) and 0. The scenario of the \(M_v,N/\Sigma_{v,N}\)’s is represented in Fig. \([6]\). We note that the \(\Sigma_v,N\)’s are not the whole border of the \(M_v,N\)’s, because the curved lines (we refer to the 2-dimensional picture) are not part of the boundary of the \(M_v\)’s. Indeed, since the potential jumps to \(+\infty\) on the curved part of the border of the \(M_v,N\)’s, the last are partially open sets. At \(v = 0\) a topological disconnection occurs. When \(v\) reaches zero from below the two innermost \((N - 1)\)-balls of the \(\Sigma_v,N\) joint becoming an \((N - 1)\)-ball alone. This is equivalent to what happens for a smooth potential when the \(v\)-level set crosses a critical level with a critical point of index 1, i.e. a saddle point. For the potential of our model the derivative along the coordinate \(m\) is negative, and the derivatives along the \(\tilde{q}_i\)’s, \(i = 1, \cdots, N - 1\), are vanishing, but the shape of the \(\Sigma_v,N\)’s can be continuously deformed in such a way to make the last derivatives positive without changing the properties of the model. We will see what just aforementioned acting in the model introduced in the next Section equipped with a smooth potential. In this case a positive shift between the critical average thermodynamic potential and the critical topological level is entailed, in contrast of the model in this Section where the last exactly coincide.

IV. MODEL OF REVOLUTION WITH SMOOTH POTENTIAL

In this Section we will see how it is possible to modify the definition of the potential of the model of the previous Section in such a way to be smooth. In that Section, after giving the definition \([7]\), we have constrained the configuration space \(M\) into an \(N\)-dimensional ‘spindle’ of size \(e^{-(N - 1)m^2}\). Here, we will follow a different way, that is, we attach at any point of the line passing through zero and orthogonal to the planes \(\pi_{m,N}\)’s a paraboloid in the coordinates \(\tilde{q}_1, \cdots, \tilde{q}_{N - 1}\) scaled by the factor \(e^{-m^2}\). In the coordinate system \([10]\) the potential is assumed to be

\[
V = N(-Jm^2 + m^4) + \sum_{i=1}^{N-1} \left(\frac{\tilde{q}_i}{e^{-m^2}}\right)^2. \tag{37}
\]

This potential has two absolute minima of value \(-\frac{NJ}{4}\) whose coordinates are \((\pm \frac{\sqrt{N}}{2}, 0, \cdots, 0)\), and has a saddle point of value 0 at \((0, \cdots, 0)\). As the model in the previous Section, this model has an \(O(N - 1)\) symmetry on the coordinates \(\tilde{q}_1, \cdots, \tilde{q}_{N - 1}\) besides the \(\mathbb{Z}_2\) one.

A. Canonical thermodynamic

The partition function is

\[
Z_N = \sqrt{N} \int dm \, d\tilde{q} \, e^{-\frac{1}{4} \left( N(-Jm^2 + m^4) + e^{2m^2} \sum_{i=1}^{N-1} \tilde{q}_i^2 \right)},
\]

which can be re-written as

\[
Z_N = \sqrt{N} \int dm \, e^{-\frac{1}{4} \left( -Jm^2 + m^4 \right)} \left( \int dq \, e^{-2m^2\tilde{q}^2} \right)^{N-1}. \tag{39}
\]

By applying the Gaussian integral formula, and for large \(N\), we get

\[
Z_N \approx \sqrt{N} \int dm \, e^{-\frac{1}{2} \left( (T - J)m^2 + m^4 - \frac{T}{2} \ln(\pi T) \right)}. \tag{40}
\]

In the thermodynamic limit, the free energy, the spontaneous magnetization, the average potential, and the specific heat are, respectively,

\[
f = (T - J)m^2 + m^4 - \frac{T}{2} \ln(\pi T), \tag{41}
\]

\[
\langle m \rangle = \begin{cases} \pm \frac{1}{\sqrt{2}}(J - T)^{\frac{1}{2}} & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c, \end{cases} \tag{42}
\]

\[
\langle v \rangle = \begin{cases} \frac{T}{2} - \frac{1}{4}(J - T^2) & \text{if } T \leq T_c, \\ \frac{T}{2} & \text{if } T \geq T_c, \end{cases} \tag{43}
\]

\[
c_v = \begin{cases} \frac{1}{2} + \frac{T}{2} & \text{if } T \leq T_c, \\ 0 & \text{if } T \geq T_c. \end{cases} \tag{44}
\]

where \(T_c = J\) is the critical temperature of the model. The SBPT is of the second order with classical critical exponents (see Fig. \([3]\) for a plot).

B. Dumbbell-shaped \(v\)-level sets at the origin of the \(\mathbb{Z}_2\)-SBPT

The topology of the \(\Sigma_{v,N}\)’s is as follows (‘\(\sim\)’ stands for ‘is homeomorphic to’)

\[
\Sigma_{v,N} \sim \begin{cases} \mathbb{S}^{N-1} & \text{if } v > 0 \\ \mathbb{S}^{N-1} \cup \mathbb{S}^{N-1} & \text{if } v = 0 \\ 0 & \text{if } 0 > v \geq -\frac{1}{4} \\ \mathbb{S}^{N-1} & \text{if } v < -\frac{1}{4}. \end{cases} \tag{45}
\]

There exists only a topological change at \(v = 0\). This potential satisfy the hypotheses of theorem 1 in \([6]\) for \(v \in [-\frac{1}{4}, 0)\), so that the \(\mathbb{Z}_2\)-SB is guaranteed for \(T \in\)
and whose volume is given by

\[ \pi v, m = \frac{2\pi^{N-1}}{\Gamma\left(\frac{N}{2}\right)} R^{N-2}. \]  

To calculate \( \omega_N(v, m) \) we should take into account the Liouville measure \( \|\nabla V\|^{-1} \), which is a function of \( v, m \) due to the \( O(N - 1) \) symmetry in the coordinates \( \hat{q}_1, \ldots, \hat{q}_{N-1} \). Following the remark in Sec. [III], we can disregard this term and replace the Liouville measure onto \( \Sigma_{v,N} \cap \pi_{m,N} \) by the standard measure induced by the embedding in \( \mathbb{R}^N \).

\( [0, T'] \), where \( T' = \langle v \rangle^{-1}(T) = -1 + \sqrt{1 + J} \) for \( \langle v \rangle = 0 \), by topological reasons. Indeed, the \( \Sigma_{v,N} \)'s are made by two disconnected components which are the image of the other under the reflection with respect to the hyperplane \( \Sigma_{0,N} \).

The critical average potential \( v_c = \frac{J}{2} \) is located above 0 which correspond to the unique critical level set. This is due to the presence of dumbbell-shaped \( \Sigma_{v,N} \)'s in the interval \([0, v_c]\). Indeed, according to theorem in [3], they imply the \( \mathbb{Z}_2 \)-SB as well as the topological disconnection.

The simplicity of this model, in particular the presence of the \( O(N - 1) \) symmetry, allows us to identify the dumbbell-shaped \( \Sigma_{v,N} \)'s by the explicit calculation of the density of states \( \omega_N(v, m) = \mu(\Sigma_{v,N} \cap \pi_{m,N}) \). Indeed, \( \Sigma_{v,N} \cap \pi_{m,N} \) is an \( (N - 1) \)-sphere defined by the following equation

\[ Nv = N(-Jm^2 + m^4) + e^{2m^2} \sum_{i=1}^{N-1} q_i^2, \]  

whose radius \( R \) is given by

\[ R^2 = \sum_{i=1}^{N-1} q_i^2 = Ne^{-2m^2} (v + Jm^2 - m^4), \]  

and whose volume is given by

\[ \text{vol} (\Sigma_{v,N} \cap \pi_{m,N}) = \frac{2\pi^{N-1}}{\Gamma\left(\frac{N}{2}\right)} R^{N-2}. \]

Anyway, \( \|\nabla V\| \) as a function of \( m, v \) vanishes at \((0, 0)\) and \((\pm \sqrt{\frac{J}{2}}, -\frac{1}{2})\), but since, when \( m \to 0 \) for \( v = 0 \), \( \|\nabla V\| \) goes to zero slower than the volume of \( \Sigma_{0,N} \cap \pi_{m,N} \), then \( \mu \to 0 \) exactly as \( \text{vol} (\Sigma_{v,N} \cap \pi_{m,N}) \). The same reasoning can be applied to the other two critical points.

By using the relation \( \Gamma\left(\frac{N-1}{2}\right) = \frac{(N-3)!!}{2^{N-1}} \sqrt{\pi} \), in the thermodynamic limit, we find out

\[ a(v, m) = \lim_{N \to \infty} \omega_N(v, m)^{\frac{1}{N}} = e^{-m^2} \sqrt{v + Jm^2 - m^4} \]  

as defined in [32]. In Fig. 6 the microcanonical entropy \( s = \ln a \) is plotted.

According to the definition given in [32], a \( \Sigma_{v,N} \) is called dumbbell-shaped if the related \( a(v, m) \), or equivalently

---

**FIG. 4:** Model of revolution with smooth potential in Sec. [IV] for \( J = 1 \). From left to right and from top to bottom: spontaneous magnetization \( \langle m \rangle \), free energy \( f \), average potential \( \langle v \rangle \), specific heat \( c_v \) versus temperature \( T \).

**FIG. 5:** Left: some \( \Sigma_{v,N} \)'s for \( N = 2 \) of the model of revolution with smooth potential in Sec. [IV] for \( v = -0.2, 0.25, 0.5, 1 \) and \( J = 1 \). \( \Sigma_{0.5,2} \) is critical in the sense that it is the boundary between the 'non-strangled' \( \Sigma_{v,N} \)'s for \( v \geq \frac{1}{2} \) and the dumbbell-shaped ones for \( -\frac{1}{2} \leq v < \frac{1}{2} \). Right: the effect of an external magnetic field \( H = 0.3 \) which breaks the \( \mathbb{Z}_2 \) symmetry.

**FIG. 6:** Model of revolution with smooth potential in Sec. [IV] for \( J = 1 \). Contour plot of the microcanonical entropy \( s(v, m) = \ln a(m) \) [32], the dark region surrounded by the curve of equation \( v = -Jm^2 + m^4 \) is the domain of \( s(v, m) \). The graphic of \( s(v, m) \) is not concave and its domain is not convex because the potential, being expressed in term of \( m \), is long-range. The imaginary horizontal line \( v = v_c = \frac{1}{2} \) is the boundary between the dumbbell-shaped \( \Sigma_{v,N} \)'s from the non-dumbbell-shaped ones.
$s(v,m)$ does not take the maximum at $m = 0$. For $v \in [-\frac{1}{4}, 0)$ the $\Sigma_{v,N}$'s are dumbbell-shaped because they are the union of two disconnected components.

Consider $v \geq 0$. To discover whether a $\Sigma_{v,N}$ is dumbbell-shaped is sufficient to set to zero the second partial derivative of $a(v,m)$ with respect to $m$ at $m = 0$

$$\frac{\partial^2 a(v,m)}{\partial m^2} \bigg|_{m=0} = 2v - J = 0,$$

whence $v = \frac{J}{2}$ is the boundary between the dumbbell-shaped $\Sigma_{v,N}$'s from that non-dumbbell-shaped. In particular, the $\Sigma_{v,N}$'s are dumbbell-shaped for $v < \frac{J}{2}$. $\Sigma_{\frac{J}{2},N}$ plays the role of critical $v$-level set. Anyway, since $\Sigma_{\frac{J}{2},N}$ is defined at finite $N$, we cannot be sure that $\Sigma_{\frac{J}{2},N}$ is just the critical level, but after some algebraic manipulations, we can show that this is just the case.

From a thermodynamic viewpoint, the critical average potential is just $v_c = \langle v \rangle(T_c) = \frac{J}{2}$. Summarizing, the thermodynamic picture of the $Z_2$-SBPT is in perfect agreement with the geometric picture of the dumbbell-shaped $\Sigma_{v,N}$ introduced in [3].

Furthermore, we note that the canonical entropy $s(v)$ can be obtained by a maximization process of $s(v,m)$ with respect to $m$, as it has been made in [22] for the mean-field $\phi^4$ model.

V. MEAN-FIELD $R^4$ MODEL

In this Section we will introduce another example of model of revolution that we call $R^4$ model. As well as the models introduced in the previous Sections, it shows in the most evident way the generating-mechanism of SBPTs based on dumbbell-shaped $v$-level sets. Consider a central potential with an $O(N)$ symmetry given by the term $|q|^4 = R^4$ multiplied by a suitable constant, where the square radius $R^2 = \sum_{i=1}^{N} q_i^2$, to which we add the mean-field Ising-like interacting term

$$V = \frac{1}{4N} \left( \sum_{i=1}^{N} q_i^2 \right)^2 - \frac{J}{2N} \left( \sum_{i=1}^{N} q_i \right)^2 = \frac{1}{4N} R^4 - \frac{NJ}{2} m^2,$$

(51)

where the factor $\frac{1}{4}$ has been inserted to guarantee $v = \frac{J}{2}$ to be intensive. This model undergoes a classical $Z_2$-SBPT. It belongs to the class of the models of revolution because the subsets at constant magnetization of the $\Sigma_{v,N}$'s are $(N-1)$-spheres, but with the advantage that the potential can be written in the standard coordinate system. Besides the mean-field version we can consider also the short-range versions of the $R^4$ model. We conjecture that the $Z_2$-SBPT occurs for any dimension $d > 2$. Mermin-Wagner theorem [37] rules out $d = 1$ and $d = 2$ because the model has a spherical symmetry which is continuous, as it is the case of the spherical model (Berlin-Kac) [2].

Let us consider the geometric-topological analysis of the potential. $\nabla V = 0$ is equivalent to the following system

$$q_i \sum_{j=1}^{N} q_j^2 - J \sum_{j=1}^{N} q_j = 0, \quad i = 1, \ldots, N. \quad (52)$$

It is easy to show that the solutions $q_i$'s for $i = 1, \ldots, N$ are all equal and that satisfy the following equation

$$q_i^3 - J q_i = 0, \quad i = 1, \ldots, N., \quad (53)$$

whence $q_i = \sqrt[3]{J}$, $q_i = -\sqrt[3]{J}$ for $i = 1, \ldots, N$. Summarizing, there are two absolute minima and a saddle. The absolute minimum value of $V$ is

$$V_{min} = -\frac{3}{4} N J^2. \quad (54)$$

The absolute minima are separated by a gap proportional to $N$, hence the $R^4$ model satisfies the hypotheses of theorem 1 in [6] for $Z_2$-SB.

A. Dumbbell-shaped $v$-level sets

$\Sigma_{v,N} \cap \pi_{m,N}$ is an $(N-1)$-sphere whose radius $r$ is linked to $R$ and $m$ via the Phytagorian theorem and the definition (51)

$$r(v,m) = \sqrt{N \left( (v + Jm^2)^{\frac{1}{2}} - m^2 \right)^{\frac{1}{2}}}, \quad (55)$$

$a_N(v,m)$ writes as

$$a_N(v,m) = C(N-1)^{\frac{1}{4}} r^{\frac{N-2}{2}}, \quad (56)$$

where $C(N-1) = \frac{2\pi^{N-1}}{\Gamma(\frac{N-1}{2})}$ which becomes as $N \to \infty$

$$a(v,m) = \left( (v + Jm^2)^{\frac{1}{2}} - m^2 \right)^{\frac{1}{2}}. \quad (57)$$
The entropy is \( s(v, m) = \ln a(v, m) \). The shape is the same of the model of the previous Section, apart the difference in the numerical values.

Now, our purpose is to find out the analytic relation between the spontaneous magnetization and the average potential, and in particular the critical average potential \( v_c \), by studying \( a(v, m) \) as a function of \( m \). Indeed, according to the theorem in [25], the \( v_c \)-level set is the boundary between the dumbbell-shaped \( v \)-levels and the non-dumbbell-shaped ones. At fixed \( v \), (hereafter, for simplicity of notation, we will make the identification \( \langle m \rangle = m \) and \( \langle v \rangle = v \)) \( m \) is related to the \( \Sigma_{v, N} \cap \pi_{m,N} \) of maximum volume, i.e. \( \frac{\partial m}{\partial m} = 0 \) at \( m(v) \), where the last function is the curve of the spontaneous magnetization as a function of the average potential. After some trivial algebraic manipulation we get the solution

\[
\frac{\partial a}{\partial m} = \frac{1}{2a(v, m)} \left( J (v + J m^2)^{-\frac{1}{2}} - 2 \right) m = 0, \tag{58}
\]

\[
m(v) = \left\{ \begin{array}{ll}
\pm \left( \frac{1}{4} + \frac{v}{J} \right)^{\frac{1}{2}} & \text{if } -v_{\min} < v \leq v_c, \\
0 & \text{if } v \geq v_c
\end{array} \right.
\]

where \( v_c = \frac{1}{4} J^2 \).

Another way for finding out \( v_c \) is setting to zero \( \frac{\partial^2 a}{\partial m^2} \) at \( m = 0 \), which after some trivial algebraic manipulation writes as

\[
\frac{\partial^2 a}{\partial m^2} \bigg|_{m=0} = \frac{1}{2} v^{-\frac{1}{2}} \left( J v^{-\frac{1}{2}} - 2 \right) = 0, \tag{60}
\]

whence the solution.

### B. Canonical thermodynamic

We cannot provide an analytical solution for this model. The presence of the SB is guaranteed by theorem 1 in [25] and the complete SBPT by the theorem in [3]. If we consider also the short-range versions of the model the dimension \( n \) of the lattice enters the game. We conjecture that the model undergoes a SBPT for any \( n > 3 \), \( n = 1 \) is excluded because the minimum gap of the potential density \( v \) between the two wells tends to zero as \( N \to \infty \). For more precision, the SBPT occurs, but the critical temperature is \( T_c = 0 \). \( n = 2 \) is excluded by Mermin-Wagner theorem [53] because the model has a continuous \( O(N - 1) \) symmetry.

### VI. MEAN-FIELD \( \phi^4 \) MODEL

We recall the potential of the mean-field \( \phi^4 \) model with a \( \mathbb{Z}_2 \) symmetry

\[
V = \sum_{i=1}^{N} \left( -\frac{\phi_i^2}{2} + \frac{\phi_i^4}{4} \right) = \frac{J}{2N} \left( \sum_{i=1}^{N} \phi_i \right)^2. \tag{61}
\]

The model is known to undergo a second-order \( \mathbb{Z}_2 \)-SBPT with classical critical exponents.

In [25] the authors have been able to calculate the thermodynamic limit of the microcanonical entropy \( s(v, m) \) by large deviations theory. The canonical entropy \( \hat{s}(v) \) is obtained by a process of maximization of \( s(v, m) \) with respect to \( m \)

\[
\hat{s}(v) = \max_{m} s(v, m). \tag{62}
\]

The domain of \( s(v, m) \) is a non-convex subset of the plane \( (v, m) \), and \( s(v, m) \) is a non-concave function, coherently with the long-range interaction of the potential. The critical average potential \( v_c \) of the SBPT is located in such a way to divide the concave subsets \( s(v, m) \) at fixed \( v \geq v_c \) from the non-concave ones at \( v < v_c \). The graphs of \( s(v, m) \) (Fig. 5 in [25] and Fig. 2 in [25]) is qualitatively identical to the one of the model in Sec. IV (Fig. 9).

In [2, 32] the topology of the \( \Sigma_{v, N} \)'s has been exhaustively studied by means of Morse theory [33]. The following three cases have been delineated:

(i) \( v \in [v_{\min}, v_t] \), where \( v_{\min} = -\frac{1}{4}(1 + J)^2 \) is the absolute minimum of the potential. \( v_t \) depends on the coupling constant \( J \), and \( v_t < -\frac{1}{4} \). The \( \Sigma_{v, N} \)'s are homeomorphic to the union of two disjoint \( N \)-spheres. The critical potential of the SBPT may be less than 0, but \( v_c > v_t \) holds for every \( J \).

(ii) \( v \in [v_t, 0] \). There is a huge amount of critical points growing as \( e^N \) as a consequence of the topological changes. We can say that the whole interval \( [v_t, 0] \) plays the role of a critical \( v \)-level set, because it discriminates between the \( \Sigma_{v, N} \)'s homeomorphic to two disjoint \( N \)-spheres from the ones homeomorphic to a \( N \)-sphere alone. In a future paper we will see how it is possible to reduce this critical interval to a single critical \( v \)-level set containing a critical point alone. Furthermore, as \( J \to \infty \), \( v_t \to -\frac{1}{4} \).

(iii) \( v \in (0, +\infty) \). The \( \Sigma_{v, N} \)'s are homeomorphic to an \( N \)-sphere.

Let us try to interpret this scenario in the framework of the dumbbell-shaped \( \Sigma_{v, N} \)'s. In the case (i) the hypotheses of theorem 1 in [25] are satisfied, thus the topology of the \( \Sigma_{v, N} \)'s implies the \( \mathbb{Z}_2 \)-SB. This is in accordance with \( v_c > v_t \) for every \( J \), because the magnetization cannot vanish below \( v_t \). As showed in Sec. IIIA of [3], since the theorem in [6] is a particular case of that given in Sec. III of [25], also the hypotheses of the latter are satisfied.

In the case (ii) the hypotheses of the theorem in [6] are not satisfied, so that only the theorem given in Sec. III of [3] can implies the \( \mathbb{Z}_2 \)-SB because the \( \Sigma_{v, N} \)'s may be dumbbell-shaped below \( v_c \) and non-dumbbell-shaped above \( v_c \) (if \( v_c < 0 \)) independently on their intricate topology.

Finally, the same of the case (ii) holds for the case (iii), with the non-significant difference that the \( \Sigma_{v, N} \)'s are all diffeomorphic to an \( N \)-sphere.
\( \Sigma_{v_c,N} \) plays the role of the critical \( v \)-level set in the sense that it separates the dumbbell-shaped \( \Sigma_{v_c,N} \)'s from the non-dumbbell-shaped ones. In general, for more precision, we aspect that at fixed \( N \) the critical \( \Sigma_{v,N} \) in the above-specified sense is not located exactly at \( v_c \), but there may exist a sequence of critical \( \Sigma_{v_c,N} \) such that \( v_c^N \rightarrow v_c \) for \( N \rightarrow \infty \). Further analytic and numerical studies may check this conjecture.

The potential of the mean-field \( \phi^4 \) model has the characteristics pointed out in [3, 4], i.e. a mean-field-like interacting potential that by the addition of a constraint given by the quartic local potential generates a double-well potential sufficient to entail the SBPT. The presence of the SBPT dose not depend on the details of the constraint, which has to satisfy only the condition \( V \rightarrow +\infty \) as the coordinates \( \phi_i \rightarrow \pm \infty \). The universality class of the SBPT is determined by the exponent of the interacting potential, in our case it is 2, that corresponds to the universality class of the classical SBPTs.

VII. CONCLUSIONS

In the recent paper [8] it has been showed a theorem according to which dumbbell-shaped \( v \)-level sets of the potential are necessary and sufficient condition to entail a \( \mathbb{Z}_2 \)-SBPT for a Hamiltonian system. Roughly speaking, a \( v \)-level set is dumbbell-shaped if it is made by too major component connected by a shrink neck. This kind of subset of configurational space can be entailed by a double-well potential.

In this paper they have been introduced some Hamiltonian models with double-well potential in order to enlighten in the clearest way the generating-mechanism of a \( \mathbb{Z}_2 \)-SBPT based on dumbbell-shaped \( v \)-level sets.

The models introduced in Sec. [III, IV] have the limitation that the potential cannot be written as an explicit function of coordinates. This limit has been overcome in the model introduced in Sec. [V] We have not been able to find any analytic solution of the thermodynamic for this model, so further studies on this direction may be desirable beside to numerical investigation too.

In Sec. [VI] the results for the mean-field \( \phi^4 \) model founded out in [1, 4, 6] have been interpreted here at the light of this new scenario. In particular we have hypothesized that the critical potential is in correspondence of a critical \( v_c \)-level set in the sense aforementioned.

It is desirable that this approach to SBPTs may be enlarged to other symmetry groups beside \( \mathbb{Z}_2 \).

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