Saddle index properties, singular topology and its relation to thermodynamic singularities for a $\phi^4$ mean field model

D. A. Garanin and R. Schilling
Institut für Physik, Johannes-Gutenberg-Universität, D-55099 Mainz, Germany

A. Scala
Dipartimento di Fisica, Universit di Roma “La Sapienza” and Center for Statistical Mechanics and Complexity, INFN Roma 1, Piazzale Aldo Moro 2, 00185 Roma, Italy

(Dated: 31 March 2004, revised 29 June 2004)

We investigate the potential energy surface of a $\phi^4$ model with infinite range interactions. All stationary points can be uniquely characterized by three real numbers $\alpha_+, \alpha_0, \alpha_-$ with $\alpha_+ + \alpha_0 + \alpha_- = 1$, provided that the interaction strength $\mu$ is smaller than a critical value. The saddle index $n_s$ is equal to $\alpha_0$ and its distribution function has a maximum at $n_s^{\text{max}} = 1/3$. The density $p(e)$ of stationary points with energy per particle $e$, as well as the Euler characteristic $\chi(e)$, are singular at a critical energy $e_c(\mu)$, if the external field $H$ is zero. However, $e_c(\mu) \neq \nu_c(\mu)$, where $\nu_c(\mu)$ is the mean potential energy per particle at the thermodynamic phase transition point $T_c$. This proves that previous claims that the topological and thermodynamic transition points coincide is not valid, in general. Both types of singularities disappear for $H \neq 0$. The average saddle index $\bar{n}_s$ as function of $e$ decreases monotonically with $e$ and vanishes at the ground state energy, only. In contrast, the saddle index $n_s$ as function of the average energy $\bar{e}(n_s)$ is given by $n_s(\bar{e}) = 1 + 4\bar{e}$ (for $H = 0$) that vanishes at $\bar{e} = -1/4 > \bar{e}_0$, the ground state energy.

PACS numbers: 05.70.Fh, 61.20.Gy, 64.70.Pf

I. INTRODUCTION

Topological features play an important role in several branches of physics. Examples in condensed matter physics are discussed in Ref. [1]. Those examples do not include thermodynamics and phase transitions. That topological concepts might be relevant for equilibrium phase transitions has already been emphasized long time ago [2] and that they can be very useful in condensed matter physics has been demonstrated recently [3, 4].

Usually, equilibrium phase transitions are indicated by a singularity at the transition temperature $T_c$ of thermodynamic quantities, like free energy, specific heat, etc. One may ask whether other indications for such phase transitions really exist. This question has been studied by several groups in recent years. Geometrical entities like the Ricci curvature, and dynamical ones like Lyapunov exponents were used for a classical planar Heisenberg model with nearest neighbor interactions and dimension $d = 2, 3$ [5], a nearest-neighbor $\phi^4$ model for $d = 3$ with $O(n)$-symmetry ($n = 1, 2, 4$) [6] and in $d = 1, 2$ with $O(1)$-symmetry [7]. It has been found that both quantities exhibit a singularity at a critical energy per particle, $e_c$, for those dimensions for which an equilibrium phase transition occurs at $T_c > 0$. Furthermore, $\nu_c$, the internal energy per particle at $T_c$, equals $e_c$, i.e., the geometrical and thermodynamic singularity occur at the same energy. It has also been speculated [3] that these singularities are related to qualitative changes in the topology of the potential energy surface (PES) of those models. That this is true indeed has been proven first for a mean-field XY-model [8].

One of the most interesting topological quantities is the Euler characteristic $\chi$ [3, 4, 5] which is a topological invariant. For the two-dimensional nearest neighbor $\phi^4$ model [10], the mean-field XY [11] and mean-field trigonometric model [12, 13] it was proven that $\chi(e)$ also becomes singular at $e_c = \nu_c$. In addition, it was shown [12, 13] that the type of singularity depends on the order of the phase transition.

$\chi(e)$ is directly related to $M(e, N_s)$, the number of stationary points of the PES of a $N$-particle system with energy $\leq e$ and saddle index $n_s = N_s/N$, by

$$\chi(e) = \sum_{N_s=0}^N (-1)^{N_s} M(e, N_s).$$

(1)

$N_s$ is the Morse index, i.e., the number of negative eigenvalues of the corresponding Hessian matrix of a stationary point. $M(e, N_s)$ is an exponentially large number in $N \gg 1$:

$$M(e, N_s) \sim \exp[N s(e, n_s)],$$

(2)

where $s(e, n_s)$ is the configurational entropy per particle. The corresponding density of states $p(e, n_s)$ is given by

$$p(e, n_s) = \frac{\partial}{\partial e} M(e, N_s) \sim \exp[N s(e, n_s)].$$

(3)

The relationship between Eqs. (1) and (2) leads to the assumption that the singularity of $\chi(e)$ may originate from a specific behavior of $p(e, n_s)$ for $N \to \infty$ or that of $s(e, n_s)$.

The density of states $p(e, n_s)$ plays an important role in the investigation of the PES. For instance, one can
define the average saddle index for a fixed energy
\[ \bar{n}_s(e) = \int_0^1 dn_s n_s p(e, n_s) \] (4)
and the average energy for a fixed value of \( n_s \)
\[ \bar{e}(n_s) = \int_{-\infty}^{\infty} de e p(e, n_s). \] (5)

In the limit \( N \to \infty \) the averages \( \bar{n}_s(e) \) and \( \bar{e}(n_s) \) are simply the values that maximize the configurational entropy, i.e., they are solutions of the equations
\[ \frac{\partial s}{\partial n_s}(e, \bar{n}_s) = 0, \quad \frac{\partial s}{\partial e}(\bar{e}, n_s) = 0. \] (6)

The saddle index properties of a PES have also played an important role in another respect. Studying glassy dynamics and ideal dynamical glass transition \cite{14} for liquids it has been found numerically \cite{15, 16} that the temperature-dependent average saddle index practically vanishes at a temperature \( T^* \), which is close to the mode-coupling glass transition temperature \( T_c \). However, this conclusion should be taken with some care. First of all most saddle points were quasi saddles (see the discussion in Refs. \cite{17, 18, 19}) and second, plotting \( \log \bar{n}_s(T) \) (or a related quantity) versus \( 1/T \) does not exhibit a quasi singular behavior at \( T_c \). \cite{20, 21}. That \( \bar{n}_s(T) \) vanishes at \( T = 0 \) only, has been proven for the \( k \)-trigonometric model \cite{12}. This indicates that \( \bar{n}_s(T) \) for systems with self-generated disorder behaves differently than for systems where the disorder is quenched. For the latter it has been proven that \( \bar{n}_s(T) \) vanishes at the dynamical transition point, at least for mean field like models \cite{22}.

A numerical determination of the true saddles of a binary liquid with particle number \( N \leq 13 \) gives evidence that \( \bar{n}_s(e) \) vanishes at an energy \( e^* \), which still depends on \( N \). \cite{17}. This evidence holds for both cases where the average \( \bar{n}_s \) is plotted versus \( e \) and \( n_s \) is plotted versus \( \bar{e} \). \cite{17}. Whether this vanishing at \( e^* \) is spurious or not is not known. It is obvious why vanishing of \( \bar{n}_s \) at \( T^* \) or \( e^* \) may be relevant. In that case, the system is mostly close to local minima \( (n_s = 0) \) for \( T < T^* \) or \( e < e^* \) and the dynamics is dominated by activated processes, in contrast to \( T > T^* \) or \( e > e^* \), where the particles dynamics is more flow-like. Hence, vanishing of \( \bar{n}_s(e) \) may indicate a qualitative change in the dynamics \cite{14, 16}.

There is another result presented in Ref. \cite{17} which concerns the distribution function of the saddle index \( p(n_s) \):
\[ p(n_s) = \int_{-\infty}^{\infty} de p(e, n_s). \] (7)
It is found that \( p(n_s) \) is a Gaussian with a maximum at \( n_s^{\text{max}} \approx 1/3 \). Although the physical relevance of this result is not clear, it seems to be an interesting property of the topology of the PES.

We hope that the exposition above has made obvious the role of topological features for both the thermodynamic and dynamic behavior. It is the main purpose of our paper to analytically investigate for a mean-field \( \phi^4 \) model the existence of a singularity in the topology of its PES and the relation to a thermodynamic singularity and to calculate the saddle index properties discussed above.

The outline is as follows. The mean-field \( \phi^4 \) model and its basic properties will be discussed in the Sec. II. In Sec. III we will investigate the topological properties of the model. In particular, we will prove that the claim that topological and thermodynamic transition points coincide is not correct, in general. The final section contains discussion where we explain the origin of this discrepancy. Some more technical details are given in the Appendix.

II. MEAN-FIELD \( \phi^4 \) MODEL

Let \( x_n \) be a scalar displacement of a particle from a lattice site \( n \). We consider the following potential energy
\[ V(x, H) = \sum_{n=1}^{N} V_0(x_n, H) - \frac{\mu}{2N} \left( \sum_{n=1}^{N} x_n \right)^2 \] (8)
depending on the \( N \)-particle configuration \( x = (x_1, \ldots, x_N) \). \( V_0(x, H) \) is an asymmetric on-site potential:
\[ V_0(x, H) = -xH - \frac{1}{2}x^2 + \frac{1}{4}x^4 \] (9)
that becomes symmetric for \( H = 0 \). The final term in Eq. \cite{9} represents the harmonic interaction between all particles with a coupling parameter \( \mu \geq 0 \). The reader should note that the potential energy and the displacement can always be scaled such that \( V_0(x, H) \) has the \( x \)-dependence given in Eq. \cite{9}. This type of models was used to describe structural phase transitions \cite{23}. In contrast to the mean-field models studied in Refs. \cite{8, 11, 12, 13} there is a nontrivial coupling constant \( \mu \), which can not be put to one by an appropriate scaling of the temperature.

Some thermodynamic properties of the model described by Eqs. \cite{8, 9} as well as some features of its PES were already investigated \cite{24}. Let us recall these results and start with the thermodynamic behavior. Due to the infinite-range interaction the mean-field approximation becomes exact for \( N \to \infty \). This leads to the self-consistency equation for the order parameter \( \langle x \rangle = \langle x_n \rangle (T, H) \):
\[ \langle x \rangle = \frac{1}{Z} \int_{-\infty}^{\infty} dx \exp \left[ -\frac{V_0(x, H) - \mu \langle x \rangle x}{T} \right], \] (10)
where $Z$ is the corresponding partition function and $\beta = 1/T$. Of course, a phase transition (second order) occurs at some $T_c$ for $H = 0$, only. $T_c$ follows from:

$$T_c = \mu \frac{\int_{-\infty}^{\infty} dx x^2 \exp \left[-V_0(x,0)/T_c\right]}{\int_{-\infty}^{\infty} dx \exp \left[-V_0(x,0)/T_c\right]}.$$  \hfill (11)

For $0 < \mu \ll 1$ one finds:

$$T_c(\mu) = \mu + \mathcal{O}(\mu^2)$$  \hfill (12)

which yields for the average potential energy per particle $\bar{V}(T) = \lim_{N \to \infty} N^{-1}\langle V(x) \rangle$ at $T_c$

$$\bar{v}_c = v(T_c) = -\frac{1}{4}(1 - 2\mu) + \mathcal{O}(\mu^2)$$  \hfill (13)

which is always larger than the minimum value $-1/4$ of $V_0(x,0)$.

Let us now turn to the stationary points as discussed in Ref. 24. With the “internal” field

$$H_{\text{int}} = \frac{\mu}{N} \sum_{n=1}^{N} x_n$$  \hfill (14)

the solution of $\partial V/\partial x_n$ reduces to that of

$$x^3 - x - H_{\text{eff}} = 0$$  \hfill (15)

with the effective field

$$H_{\text{eff}} = H + H_{\text{int}}.$$  \hfill (16)

For $|H_{\text{eff}}| < H_c = 2/(3\sqrt{3})$ there are three real roots of Eq. (15) which will be denoted by $x_{+}(H_{\text{eff}})$, $\sigma = +, 0, -$. It is $x_+ > x_0 > x_-$. A stationary point of $V$ is characterized by $N_{\sigma}$, the number of $x_n$ in $\mathbf{x}$ which are equal to $x_{+}(H_{\text{eff}})$. Permuting the particle indices yields stationary points with the same potential energy. Since $\{x_n\}$ are displacements and not positions of particles in a liquid, these permutations should be counted as different stationary points. Hence there are:

$$P(N_+, N_0, N_-) = \frac{N!}{N_+!N_0!N_-!}$$  \hfill (17)

stationary points of class $(N_+, N_0, N_-)$, where

$$\sum_{\sigma} N_{\sigma} = N,$$  \hfill (18)

i.e., $N_- = N - N_+ - N_0$. The characterization of all stationary points by $N_+, N_0$ and $N_-$ or equivalently by

$$\alpha_{\sigma} = \frac{N_{\sigma}}{N}, \sum_{\sigma} \alpha_{\sigma} = 1$$  \hfill (19)

proves (see, e.g., Sec. 3) to be extremely useful. Having specified $\alpha_{\sigma}$ we can determine $H_{\text{eff}}(\alpha_+, \alpha_0)$ from Eqs. (14) and (16):

$$H_{\text{eff}} = H + \mu \sum_{\sigma} \alpha_{\sigma} x_{\sigma}(H_{\text{eff}}).$$  \hfill (20)

![Fig. 1](image-url)

**FIG. 1:** $a-\alpha_+$-dependence of $v(\alpha_+, \alpha_0)$ for $\mu = 0.2$ and $H = 0$; $b$—Same for $H = 0.1$. Dotted lines locate the maxima. Note the concavity of $v(\alpha_+, \alpha_0)$ in $\alpha_+$ for $H \geq 0$ and its symmetry with respect to the maximum position $\alpha_+^{\text{max}} = (1 - \alpha_0)/2$ for $H = 0$.

[We omit the arguments $H$ and $\mu$ for brevity and we take into account that $\alpha_-$ can be expressed by $\alpha_+, \alpha_0$, due to Eq. (19). Also we will mostly drop the arguments of $H_{\text{eff}}(\alpha_+, \alpha_0)$]. Finally the stationary points of class $(N_+, N_0, N_-)$ are given by:

$$\mathbf{x}(H_{\text{eff}}) = (x_+(H_{\text{eff}}), \cdots ; x_0(H_{\text{eff}}), \cdots ; x_-(H_{\text{eff}}), \cdots ),$$

and its permutations. Similarly for the potential energy per particle $v(\alpha_+, \alpha_0)$ follows:

$$v(\alpha_+, \alpha_0) = \sum_{\sigma} \alpha_{\sigma} V_0(x_{\sigma}(H_{\text{eff}}), H) - \frac{1}{2\mu} [H_{\text{eff}} - H]^2.$$  \hfill (21)

Fig. 1 presents $v(\alpha_+, \alpha_0)$ as a function of $\alpha_+$ for different values of the parameters.

Eq. (21) holds for $|H_{\text{eff}}| \leq H_c$. One can easily prove that the latter is guaranteed for arbitrary $\{x_{\sigma}\}$ with
where the configurational entropy is given by
\[ -H_c(1 - 3\mu) \leq H \leq (1 - 3\mu)H_c. \] (22)
This implies the necessary condition \( \mu < 1/3 \) (cf. also Ref. [24]). \( \mu = 1/3 \) is a critical value for the coupling parameter at which the PES changes qualitatively. If inequality Eq. (22) is violated, the stationary points are not uniquely classified by \( \{\alpha_s\} \). Therefore we will restrict ourselves to \( \mu \leq 1/3 \), in the following. What remains to be done is to determine the saddle index \( n_s \) of these stationary points. The answer is simple [24], because
\[ n_s \equiv \alpha_0. \] (23)
This has been proven for \( H = 0 \) in Ref. [24] by determination of the number \( N_s \) of negative eigenvalues of the Hessian at stationary configurations with \( N_0 \) fixed. The result is that \( N_s = N_0 \), which implies Eq. (24). Validity of Eq. (25) can also be seen as follows. If \( \mu = 0 \) and \( H \geq 0 \), the stationary points of \( V \) are given by those of \( V_0 \) and the sign of the eigenvalues of the Hessian equals the sign of \( V_0' \). Since \( N_0 \) is the number of particles with position \( x_0(H) \), which is on the concave part of \( V_0 \), i.e. \( V_0''(x_0(H)) < 0 \), it is \( N_0 = N_s \). \( N_s \) is a topological invariant for \( 0 \leq \mu < 1/3 \). Consequently Eq. (25) remains true for all \( \mu < 1/3 \) and all \( H \) obeying Eq. (22).

III. STATISTICS OF STATIONARY POINTS

A. Saddle index distribution

We have shown in Sec. II that all stationary states of the mean-field \( \phi^4 \) model are characterized by \( \{\alpha_s\} \), provided inequality Eq. (22) holds. \( \alpha_0 = n_s \) is the saddle index. Consequently there are in total \( 3^N \) stationary points, from which \( 2^N \) are local minima. The saddle index distribution follows from Eq. (17):
\[ p(n_s) = 3^{-N} \sum_{N_s=0}^{N-N_s} P(N_+, N_s) = \frac{3^{-N}2^{-N-N_s}N!}{N_s!(N-N_s)!} \] (24)
Using the Stirling formula for \( N \gg 1 \) one obtains
\[ p(n_s) \sim \exp [Ns(n_s)], \]
where the configurational entropy is given by
\[ s(n_s) = -\left[ n_s \ln n_s + (1 - n_s) \ln \frac{1 - n_s}{2} \right]. \] (25)

We stress that the validity of \( n_s^{\text{max}} = 1/3 \) is more general. Suppose there are no interactions. Then the \( N \)-particle problem separates into that of \( N \) independent particles in double wells, for which \( P(N_+, N_0) \) is still given by Eq. (24). Turning on an arbitrary interaction will not destroy the one-to-one correspondence between stationary points and \( (N_+, N_-, N_0) \), up to a critical interaction strength. At this critical strength, e.g., exponentially many metastable configurations may become unstable. Accordingly, \( n_s^{\text{max}} = 1/3 \) holds up to that critical coupling, i.e., it is a topological invariant.

B. Calculation of the density of states \( p(e, n_s) \)

The density of stationary points of a PES with energy \( e \) and saddle index \( n_s \) that was mentioned in the Introduction is defined by
\[ p(e, n_s) = \sum_{N_s=0}^{N-N_s} P(N_+, N_s) \delta (v(\alpha_+, \alpha_0) - e), \] (26)
where \( P(N_+, N_0) \) is given by Eq. (24) and
\[ N_0 = \alpha_0 N = n_s N, \quad N_+ = \alpha_+ N. \]
The density \( p(e) \) of stationary points with energy \( e \), follows from
\[ p(e) = \sum_{N_0=0}^{N} p(e, n_s), \] (27)
Neglecting the irrelevant prefactor one can immediately write \( (\alpha_0 = n_s) \)
\[ p(e, n_s) \sim P(N_+, e, \alpha_0), N_0, \] (28)
where \( N_+(e, \alpha_0) = \alpha_+ (e, \alpha_0) N \) follows from the solution of the equation
\[ v(\alpha_+, \alpha_0) = e. \] (29)
This equation has two solutions \( \alpha_+ (e, \alpha_0) \) which are derived and discussed in Appendix B.

With the use of the Stirling formula \( P(N_+, N_0) \) simplifies to \( P(N_+, N_0) \sim \exp [Ns(e, \alpha_0)] \), thus one obtains Eq. (27) with the configurational entropy given by
\[ s(e, \alpha_0) = -\alpha_0 \ln \alpha_0 - \alpha_+^{(+)} \ln \alpha_+^{(+)} - \alpha_-^{(-)} \ln \alpha_-^{(-)}, \] (30)
where \( \alpha_+^{(+)} = 1 - \alpha_0 - \alpha_+^{(+)} \) and we have taken the \((+)\) branch of Eq. (51) that makes the dominant contribution into \( P(N_+, N_0) \) for \( H > 0 \). For \( H = 0 \) one can also restrict oneself to \( \alpha_+^{(+)} \), due to the symmetry. Note that \( p(e, n_s) \) is nonzero and given by Eq. (29) only in the energy window
\[ v_{\text{min}}(\alpha_0) \leq e \leq v_{\text{max}}(\alpha_0), \] (31)
where \( v_{\text{min}}(a_0) = v(1-a_0, a_0) \) (see Fig. 1) and \( v_{\text{max}}(a_0) \) is given by Eq. (A7), otherwise \( p(e, n_s) = 0 \). Alternatively one can say that Eq. 3 is valid in the window of saddle indices

\[
\alpha_0^{(\text{min})}(e) \leq \alpha_0 \leq \alpha_0^{(\text{max})}(e),
\]

(32)

where the boundary values satisfy \( v_{\text{min}}(\alpha_0^{(\text{max})}) = e \) and \( v_{\text{max}}(\alpha_0^{(\text{min})}) = e \). From Eq. (A7) one finds

\[
\alpha_0^{(\text{min})}(e) = 1 + 4e - 2H^2/\mu,
\]

(33)

whereas \( \alpha_0^{(\text{max})}(e) \) can be found with the help of Eq. (21) or, approximately, with the help of Eq. (A7). The dependence of \( s(e, n_s) \) on \( n_s \) is shown in Fig. 2 for zero and nonzero field.

Let us discuss the main features of \( s(e, n_s) \) presented in Fig. 2. For a more detailed analytical discussion of \( s(e, n_s) \) the interested reader is referred to Appendix B. We begin with \( H = 0 \) (see Fig. 2). The maximum of \( s(e, n_s) \) with respect to \( n_s \) is denoted by \( \bar{n}_s(e) \). Because of the relation between \( p(e, n_s) \) and \( s(e, n_s) \) given by Eq. 3 it is obvious that for \( N \to \infty \) the maximum position \( \bar{n}_s(e) \) is identical to the averaged saddle index \( \bar{n}_s(e) \) given by Eq. 4. In Appendix B the existence of a critical energy \( e_c(\mu) \) is proven. \( s(e, n_s) \) as function of \( n_s \) has a maximum within the domain of \( n_s \) for \( e < e_c(\mu) \) and a maximum at the left border of its domain for \( e \geq e_c(\mu) \). This implies that the slope \( \partial s(e, n_s) / \partial n_s \) at \( n_s(e) \) is continuous in \( e \), but not differentiable, i.e., the “curvature” \( \partial^2 s(e, n_s) / \partial n_s^2 \) is discontinuous in \( e \) at \( e = e_c(\mu) \). This is the origin of the topological singularity, discussed below. Fig. 3a presents \( \bar{n}_s(e) \) and reveals the singularity at \( e_c(\mu) \). Note that \( \bar{n}_s(e) \) contains a branch that is independent of the interaction [see Eqs. (13) and (14)]. For \( e \) very close to the ground state energy \( v_0(\mu) \) [cf. (20)] one obtains the power-law behavior (see Appendix B):

\[
\bar{n}_s(e) \sim [e - v_0(\mu)]^{\delta(\mu)}
\]

(34)

with \( \delta(\mu) > 1 \), if \( \mu \) is small enough. Note that \( \bar{n}_s(e) \to 0 \) for \( e \to v_0(\mu) \). The averaged saddle index \( \bar{n}_s(e) \) takes the critical value \( n_s(c)(\mu) = \bar{n}_s(e_c(\mu)) \) shown in Fig. 3. This figure also includes the asymptotic result of Eq. (15) for \( \mu \to 0 \).

Instead of fixing \( e \), one can also determine the maximum position \( c(n_s) \) of \( s(e, n_s) \) for given \( n_s \). \( c(n_s) \) is the

FIG. 2: \( a \) – Configurational entropy \( s(e, n_s) \) versus \( n_s \) for different energies and zero field; \( b \) – same for nonzero field.

FIG. 3: \( a \) – Averaged saddle index \( \bar{n}_s(e) \) versus \( e \) for \( \mu = 0.1, 0.2, 1/3 \) and \( H = 0 \); \( b \) – Same for \( \mu = 0.2 \) and \( H = 0 \) and \( H = 0.15 \).
averaged saddle energy [cf. Eq. (36)] as function of $n_s$. It is easy to get $\bar{e}(n_s)$, since the number of stationary configurations is maximal for $\alpha_+ = \alpha_- = (1-n_s)/2$. This yields for the effective field $H_{\text{eff}}(\alpha_+ = (1-n_s)/2, \alpha_0 = n_s) = 0$ which implies $x_\pm(\alpha_+ = (1-n_s)/2, \alpha_0 = n_s) = \pm 1$ and $x_0(\alpha_+ = (1-n_s)/2, \alpha_0 = n_s) = 0$ and this in turn leads to

$$\bar{e}(n_s) \equiv v(\alpha_+ = (1-n_s)/2, \alpha_0 = n_s) = -(1-n_s)/4.$$  \hfill (35)

The reader should note that (i) the inverse function $n_s(\bar{e})$ (see Fig. 6) of $\bar{e}(n_s)$ turns to zero at $\bar{e} = -1/4$ which equals the lowest energy of the on-site potential, but is above the ground state energy $v_0(\mu)$ and (ii) $\bar{e}(n_s)$ is not the inverse of $\bar{n}_s(e)$. This difference is related to the fact that the maximum of $p(e, n_s)$ with respect to $n_s$ for fixed $e$ is not generally related to its maximum with respect to $e$ for fixed $n_s$.

Now let us take $H \neq 0$ (see Fig. 3b). As discussed in Appendix B, $s(e, n_s)$ has always a maximum at $\bar{n}_s(e)$ as function of $n_s$ within its domain. $\bar{n}_s(e)$ is shown in Fig. 3a. The nonsingular $e$-dependence for $H \neq 0$ can clearly be seen. The average energy $\bar{e}(n_s)$ or its inverse $n_s(\bar{e})$ can be derived analytically (see Appendix B). The result for $n_s(\bar{e})$ is shown in Fig. 3.

Having determined $\bar{n}_s(e)$ for $H = 0$ and $H \neq 0$, one can now calculate the energy-dependent configurational entropy that follows from Eq. (27), in the limit $N \to \infty$

$$s(e) = s(e, \bar{n}_s(e)).$$  \hfill (36)

The result is shown in Fig. 5. As can be seen from Fig. 5, $s(e)$ has a discontinuous second derivative for $H = 0$ at $e = e_c(\mu)$. In Fig. 4 these points are marked by circles. The high-energy branch of $s(e)$ has the form of Eq. (25) with $\bar{n}_s(e) \to 1 + 4e$. It attains a maximum for $\bar{n}_s(e) = 1/3$ that implies $e = -1/6$, independently of the interaction.

FIG. 4: $\mu$-dependence of the critical average saddle index $n^{(c)}(\mu)$ for $0 \leq \mu \leq 1/3$ (solid line). The dashed line is the asymptotic result Eq. (16) for $\mu \ll 1$.

FIG. 5: Saddle index $n_s(\bar{e})$ versus averaged energy $\bar{e}$ for $\mu = 0.2$ and $H = 0$ and 0.15.

C. Euler characteristic $\chi(e)$

It turns out that for the model under consideration in the limit $N \to \infty$ the Euler characteristic of Eq. (11) satisfies

$$|\chi(e)| \sim p(e), \quad \frac{1}{N} \ln |\chi(e)| = s(e).$$  \hfill (37)

Calculation of $\chi(e)$ for large $N$ is similar to that of $s(e)$, as suggested by the similar form of Eqs. (2) and (3). The only difference is that $M(e, N_s)$ used in the calculation of $\chi(e)$ is, unlike $p(e, n_s)$, nonzero for $v_{\text{max}}(\alpha_0) < e$. In this case it is independent of the energy and has the form

$$M(N_s) = \frac{2^{N-N_s} N!}{N_s!(N-N_s)!},$$  \hfill (38)

similar to Eq. (24). Hence there are two different contributions into $\chi(e)$. It can be easily shown that the contribution from the range $v_{\text{min}}(\alpha_0) < e < v_{\text{max}}(\alpha_0)$ for $N \to \infty$ coincides with that of $p(e) \sim \exp[N s(e)]$ that was studied above up to an irrelevant prefactor, in spite of the sign alternation in Eq. (11). In contrast, the contribution from the range of $N_s$ determined by $v_{\text{max}}(\alpha_0) < e$ is dominated not by the maximum of $M(N_s)$ on $N_s$ but by $N_s$ on the boundary of its interval, i.e., by $N_s$ satisfying $v_{\text{max}}(N_s/N_s) = e$. One can easily see that this contribution to $\chi(e)$ never exceeds that from the range $v_{\text{min}}(\alpha_0) < e < v_{\text{max}}(\alpha_0)$, thus one obtains $|\chi(e)| \sim p(e)$ for $N \to \infty$.

The reason for such a peculiar behavior of the contribution from the range $v_{\text{max}}(\alpha_0) < e$ is the sign alternation in $\chi(e)$ plus the specific form of $M(N_s)$. For instance, as all stationary points are below the level $e = 0$, one finds $\chi(e)$ for $e > 0$, by just summing over all $N_s$:

$$\chi(e > 0) = \sum_{N_s=0}^N (-1)^N M(N_s) = 1.$$
We have shown that the distribution of the saddle indices \( p(n_s) \), where \( n_s = N_s/N \) and \( N_s \) is the number of unstable directions at a stationary point has a maximum at \( n_s = n^\text{max}_s = 1/3 \). Interestingly this value is consistent with that found for small binary Lennard-Jones clusters \([17]\). Whether or not this is an accident is not clear. Our result originates from the fact that all stationary points can be labelled by symbolic sequences \((\sigma_1, \cdots, \sigma_n)\) with \( \sigma_n = +, 0, - \). The low-temperature anomalies of structural glasses are usually explained by the existence of two-level systems arising from an ensemble of double-well potentials. As the smallest “unit” of a PES of a classical \( N \)-particle system, one may choose the local minima including their basins of attraction. But such a choice does not fully encompass the saddle. Taking the next larger unit, a pair of local minima and their common saddle, one arrives at a double-well characterization of the PES. This could explain why \( n^\text{max}_s = 1/3 \) for small clusters and for liquids. We have also argued that the value \( n^\text{max}_s = 1/3 \) is a topological invariant for an entire family of \( \phi^4 \) models. In any case, it would be important to determine \( n^\text{max}_s \) for other e.g., liquid-like models and to check whether it equals again \( n^\text{max}_s = 1/3 \).

For our model the absolute value of the Euler characteristic \( \chi(e) \) is essentially the same as the density of stationary points \( p(e) \) in the limit \( N \to \infty \), see Eq. (13). It would be interesting to investigate the generality of this result.

For \( H = 0 \) we have found a singularity in \( p(e) \) and thus in \( |\chi(e)| \) at the energy \( e_c(\mu) \) given by Eq. (15). \( e_c(\mu) \) is nonanalytic in \( \mu \). At \( e = e_c(\mu) \) the second derivative \( d^2 \ln |\chi(e)|/de^2 \) is discontinuous, as found for the models studied in Refs. [10, 11, 12, 13]. In agreement with these papers, we also have found that the topological singularity disappears for nonzero field, as well as the thermodynamic singularity. In this respect, we would like to mention a recent publication Ref. [27], where it is proven that a topological singularity is a necessary condition for a thermodynamical transition to take place. However, at variance with earlier work [10, 11, 12, 13], this singularity is not related to the thermodynamic singularity of our model as \( e_c(\mu) \) does not coincide with \( v_c(\mu) \), the average potential energy at temperature \( T_c/\mu \).

The reasons for this discrepancy can be made clear with the help of the following argument. Let us smoothly modify the local potential \( V_0(x) \) in the intervals \([-\infty, -1 - \varepsilon(\mu)]\), \([-1 + \varepsilon(\mu), -\varepsilon(\mu)]\), \([\varepsilon(\mu), 1 - \varepsilon(\mu)]\) and \([1 + \varepsilon(\mu), \infty]\) for \( 0 < \varepsilon(\mu) < 1 \). If \( \mu \) is small enough, which implies that the internal field is small enough, then the three roots of Eq. (13) are within the intervals \([\sigma - \varepsilon(\mu), \sigma + \varepsilon(\mu)]\), \( \sigma = +, 0, - \), in which the potential has not been modified. Accordingly, the roots and therefore the stationary points and their energies are the same. This implies that \( e_c(\mu) \) is the same. However, since the calculation of \( T_c(\mu) \) [cf. Eq. (11)] involves \( V_0(x) \) for all \( x \), the critical temperature will be different for the modified on-site potential.

The discrepancy between the topological and thermo-
dynamic singularities can also be traced back to an unjustified comparison of a continuous model (thermodynamics) and a discrete model (topology). More logically, the energy of all the stationary points can be represented by an Ising-like Hamiltonian \( \mathcal{H}(\{\sigma_i\}) \) (for \( \mu < 1/3 \)) with \( \sigma_i = +, 0, - \). The corresponding canonical partition function \( Z(T) = \text{Tr} \exp[-\mathcal{H}(\{\sigma_i\})] \) can be calculated from the density of states \( p(e) \) as

\[
Z(T) = \int p(e) \exp[-Ne/T].
\]  

(39)

Evidently a singularity of \( Z(T) \) at the corresponding transition temperature \( T'_c \) results from the underlying singularity of \( p(e) \) at \( e_c \). Obviously in this case \( v'_e(\mu) = (\mathcal{H}(T'_c))/N = e_c(\mu) \) is fulfilled. But the thermodynamics of this discrete model does not coincide with that of the original continuous model, in particular, \( T'_c \neq T_c \).

The idea of an at least qualitative relationship between the thermodynamic singularity and the topological singularity is supported by the following observation. At the thermodynamic transition point there appears a spontaneous breaking of the left-right symmetry for the displacements, which is equivalent to emerging of a nonzero temperature-dependent internal field for \( T < T_c(\mu) \). On the other hand, the stationary configurations with \( e > e_c(\mu) \) and with maximum weight correspond to \( \alpha_+ = \alpha_- \). This implies that the effective field defined by Eqs. (14) and (15) satisfies \( H_{eff} = 0 \). However for \( e < e_c(\mu) \) it is \( \alpha_+ \neq \alpha_- \) and hence \( H_{eff} \neq 0 \). Therefore a spontaneous symmetry breaking occurs at both singularities.

The energy- temperature-dependence of the averaged saddle index \( n_s \) seems to play a role for the dynamical features of supercooled liquids. For the present model we have found that \( n_s(e) \) vanishes at the ground state energy \( \nu_0 \), only. This is consistent with recent results on \( n_s(T) \) showing that \( n_s = 0 \) at \( T = 0 \), only \[15\]. Taking the analogy to mean-field like spin glass models, this would imply that no dynamical transition (or crossover) could occur at finite temperatures \[22\]. The averaged energy \( \bar{e}(n_s) \) as function of \( n_s \) is not the inverse function of \( n_s(e) \). In particular \( n_s(\bar{e}) \) vanishes at \( e^*(H) > \nu_0 \). Whether dynamics changes qualitatively at \( e^*(H) \) or any other characteristic temperature would be interesting to study.

Finally we would like to mention that after submission of this paper we learned about a similar study of the same model \[25\], where the authors find, among others, the same type of discrepancy between the thermodynamical and topological singularities.

**APPENDIX A: PROPERTIES OF \( v(\alpha_+, \alpha_0) \)**

In this Appendix we investigate the properties of \( v(\alpha_+, \alpha_0) \) defined by Eq. (21). For the discussions in Sec. 3, the first and second derivative of \( v(\alpha_+, \alpha_0) \) with respect to \( \alpha_+ \) will be useful. A straightforward calculation making use of Eqs. (15), (16) and (20) yields:

\[
\frac{\partial v(\alpha_+, \alpha_0)}{\partial \alpha_+} = V_0(x_+(H_{eff}), H_{eff}) - V_0(x_+(H_{eff}), H_{eff}).
\]

(A1)

Since \( H_{eff} = 0 \) implies \( x_\pm = \pm 1 \) [see Eq. (15)] it follows that \( \partial v(\alpha_+, \alpha_0)/\partial \alpha_+ = 0 \) for \( H_{eff} = 0 \). That is, the maximum of \( v(\alpha_+, \alpha_0) \) with respect to \( \alpha_+ \) corresponds to \( H_{eff} = 0 \). For the second derivative we get:

\[
\frac{\partial^2 v(\alpha_+, \alpha_0)}{\partial \alpha_+^2} = -[x_+(H_{eff}) - x_-(H_{eff})] \times \frac{\partial H_{eff}(\alpha_+, \alpha_0)}{\partial \alpha_+}.
\]

(A2)

with

\[
\frac{\partial H_{eff}(\alpha_+, \alpha_0)}{\partial \alpha_+} = \frac{x_+(H_{eff}) - x_-(H_{eff})}{1 - \mu \sum_{\sigma} n_s(\sigma)}.
\]

(A3)

Since \( x_+ - x_- > 0 \), the “curvature” \( \partial^2 v/\partial \alpha_+^2 \) is negative, i.e., \( v(\alpha_+, \alpha_0) \) is concave in \( \alpha_+ \), provided \( \partial H_{eff}/\partial \alpha_+ > 0 \). This is true if \( \mu \) is small enough, as can be seen from Eq. (A3).

The function \( v(\alpha_+, \alpha_0) \) can be computed analytically near its minimum in \( \alpha_+ \) by using the expansions

\[
x_-(H_{eff}) \approx -1 + H_{eff}/2,
\]

\[
x_+(H_{eff}) \approx 1 + H_{eff}/2,
\]

(A4)

near \( H_{eff} = 0 \). The result is a parabola in \( \alpha_+ \):

\[
\hat{v}(\alpha_+, \alpha_0) \approx -\frac{1}{4} (1 - \alpha_0) + \frac{H_{eff}^2}{2\mu} - \frac{1}{2\mu} \left[ H + \mu (2\alpha_+ + \alpha_0 - 1) \right]^2.
\]

(A5)

Analysis shows that corrections to this formula in the whole region \( 0 \leq \alpha_+ \leq 1 - \alpha_0 \) are of order \( \mu^3, \mu^2 H, \) and \( \mu H^2 \), i.e., Eq. (A5) is a very good approximation for not too large \( \mu \). For instance, the ground-state energy following from Eq. (A5) in the case \( H = 0 \)

\[
\hat{v}_0(\mu) = \hat{v}(0,0) = -\frac{1}{4} \left( 1 + \frac{2\mu}{1 - \mu/2} \right)
\]

is in accord with the exact two-fold degenerate ground-state energy,

\[
v_0(\mu) = v(1,0) = v(0,0) = -\frac{1}{4} (1 + \mu)^2.
\]

(A6)

up to the terms \( \mu^2 \), and the relative error is only 0.0125 for \( \mu = 1/3 \). The exact value of the field-dependent maximal potential energy that also follows from Eq. (A5) has the form

\[
v_{max}(\alpha_0) = -\frac{1}{4} (1 - \alpha_0) + \frac{H_{eff}^2}{2\mu}.
\]

(A7)
The corresponding exact value of $\alpha_+$ is
\[
\alpha_+^{(\text{max})}(\alpha_0) = \frac{1 - \alpha_0}{2} - \frac{H}{2\mu}. \tag{A8}
\]
Eqs. (A7) and (A8) are thus valid for $|H| \leq \mu(1 - \alpha_0)$.

**APPENDIX B: CONFIGURATIONAL ENTROPY**

In this Appendix we present analytical results for the configurational entropy $s(e, n_s)$. In particular, for $H = 0$ the existence of a critical energy $e_c(\mu)$ will be proven, at which singular energy dependence occurs.

First we have to investigate $v(\alpha_+, \alpha_0)$. It is convenient to use the approximate form of $v(\alpha_+, \alpha_0)$ given by Eq. (A8). Then Eq. (B1) becomes quadratic, and one obtains two solutions
\[
\alpha_+^{(\pm)} = \alpha_+^{(\text{max})}(\alpha_0) \\
\pm \sqrt{\frac{[v_{\text{max}}(\alpha_0) - e][1 - \mu(1 - 3\alpha_0)/2]}{2\mu}}, \tag{B1}
\]
where $\alpha_+^{(\text{max})}(\alpha_0)$ and $v_{\text{max}}(\alpha_0)$ are given by Eqs. (A8) and (A7), respectively. Note that this result becomes exact for all $\mu$ with $0 < \mu \leq 1/3$ provided that $e$ is close to $v_{\text{max}}(\alpha_0)$.

The value of $\bar{n}_s(e)$ that maximizes the entropy $s(e, \alpha_0)$ on $\alpha_0$ is the solution of the equation
\[
\frac{\partial \alpha_+^{(\pm)}}{\partial \alpha_0} \ln \frac{1 - \alpha_0 - \alpha_+^{(\pm)}}{\alpha_+^{(\pm)}} + \ln \frac{1 - \alpha_0 - \alpha_+^{(\pm)}}{\alpha_0} = 0 \tag{B2}
\]
for $\alpha_0$, if this solution exists in the interval of Eq. (B2). Otherwise the maximum of $s(e, \alpha_0)$ is attained at the left boundary of the $\alpha_0$-window, $\alpha_0 = \alpha_0^{(\text{min})}(e)$ (see Fig. 2b).

The latter solution exists only for $H = 0$. It corresponds to the maxima of the curves $v(\alpha_+, \alpha_0)$ in Fig. 1, i.e., to
\[
\alpha_+^{(\pm)} = \alpha_+^{(-)} = \alpha_+^{(\text{max})}(\alpha_0) = \frac{1 - \alpha_0}{2}. \tag{B3}
\]

One can see from Eq. (B1) that $\partial \alpha_+^{(\pm)}/\partial \alpha_0$ diverges for $e \to v_{\text{max}}(\alpha_0)$, i.e., for $\alpha_0 \to \alpha_0^{(\text{min})}(e)$. One can check that in the case $H = 0$ this divergence is compensated for by the log factor that tends to zero. For $H \neq 0$ there is no such compensation, and the lhs of Eq. (B2) diverges at $\alpha_0 \to \alpha_0^{(\text{min})}(e)$, thus Eq. (B2) always has a solution, see Fig. 2b.

Let us consider the case $H = 0$ and find the condition that the solution of Eq. (B2) is just $\alpha_0 = \alpha_0^{(\text{min})}(e)$. Simplifying this equation for $e \to v_{\text{max}}(\alpha_0)$ one obtains the transcendental equation
\[
-\frac{1 - \mu(1 - 3\alpha_0)/2}{4\mu(1 - \alpha_0)} + \ln \frac{1 - \alpha_0}{2\alpha_0} = 0. \tag{B4}
\]
Its solution $\alpha_0^{(c)}(\mu) \equiv n_s^{(c)}(\mu)$ that is plotted in Fig. 1 and the corresponding energy $e_c^{(c)}(\mu)$ are critical parameters that define the boundary between different regimes. In particular, $\alpha_0^{(c)}(1/3) \simeq 0.1774$ and $e_c^{(c)}(1/3) \simeq -0.2056$. For $\mu \ll 1$ one can solve Eq. (B4) analytically:
\[
n_s^{(c)}(\mu) = \frac{1}{2} \exp \left(-\frac{1}{4\mu}\right) \tag{B5}
\]
\[
e_c(\mu) = -\frac{1 - n_s^{(c)}(\mu)}{4} \approx -\frac{1}{4} + \frac{1}{8} \exp \left(-\frac{1}{4\mu}\right). \tag{B6}
\]
Note that $e_c^{(c)}(\mu)$ is always above $-1/4$, the ground-state energy without interaction. Now one can write down the combined expression for $\bar{n}_s(e)$ in the case $H = 0$:
\[
\bar{n}_s(e) = \begin{cases} 
\bar{n}_s^{(c)}(e), & e \leq e_c(\mu) \\
\bar{n}_s^{(\text{max})}(e), & e_c(\mu) \leq e \leq 0 \\
0, & 0 \leq e.
\end{cases} \tag{B6}
\]

Here $v_0(\mu)$ is the ground-state energy, $\bar{n}_s^{(c)}(e)$ is equal to $\alpha_0$ that solves Eq. (B2), and
\[
\bar{n}_s^{(\text{max})}(e) = 1 + 4e. \tag{B7}
\]

Note that the high-energy branch $\bar{n}_s^{(\text{max})}(e)$ is independent of $\mu$ and is thus the same as for a system of noninteracting particles. This contribution is due to the maxima of $v(\alpha_+, \alpha_0)$ [see Eq. (B5)] whereas $\bar{n}_s^{(c)}(e)$ is the contribution from the energy levels below this maximum. One can show that $\bar{n}_s(e) \to 0$ for $e \to v_0(\mu)$. This dependence has the form given by Eq. (B4). However this dependence is only realized for the energies very close to the ground state $v_0(\mu)$. The function $\bar{n}_s(e)$ is shown in Fig. 3 for $H = 0$ and $H \neq 0$. It has a discontinuous derivative at $e = e_c(\mu)$ in zero field. This discontinuity disappears for $H \neq 0$.

One can also use $p(e, n_s)$ to calculate the average energy $\bar{e}(n_s)$ for a given $n_s$. From the second of Eqs. (B1) one obtains
\[
\ln \frac{1 - \alpha_0 - \alpha_+^{(\pm)}}{\alpha_+^{(\pm)}} = 0
\]
that is simpler than Eq. (B2). From its solution
\[
\bar{e}(n_s) = -\frac{1 - n_s}{4} - \frac{H^2}{4} - \frac{1 - 3n_s}{1 - \mu(1 - 3n_s)/2}. \tag{B8}
\]
one obtains $n_s(\bar{e})$ shown in Fig. 4 that is almost linear in $\bar{e}$ in the considered range of parameters, Eq. (B8). Note that, in contrast to $\bar{n}_s(e)$, the quantity $n_s(\bar{e})$ found from Eq. (B8) turns to zero not at the ground-state energy but at $\bar{e} = -1/4 - H^2/(2(2 - \mu))$. 
[1] D. Thouless, *Topological Quantum Numbers in the Non-relativistic Physics*, (World Scientific, Singapore, 1998).

[2] M. Rasetti in “Differential Geometric Methods in Mathematical Physics, ed. H. D. Döbner (Springer-Verlag, New York, 1979) and in “Structural Stability in Statistical Mechanics”, ed. W. Gütlinger (Springer-Verlag, Berlin, 1979).

[3] *Statistical Physics and Spatial Statistic*, Lecture Notes in Physics, Vol. 554, eds. K. Mecke and D. Stoyan (Springer-Verlag, Berlin, 2000); *Morphology of Condensed Matter*, Lecture Notes in Physics, Vol. 600, eds. K. Mecke and D. Stoyan (Springer-Verlag, Berlin, 2002).

[4] K. Michielsen and H. De Raedt, Phys. Rep. 347, 461 (2001).

[5] L. Caiani, L. Casetti, C. Clementi and M. Pettini, Phys. Rev. Lett. 79, 4361 (1997).

[6] L. Caiani, L. Casetti, C. Clementi, G. Pettini, M. Pettini and R. Gatto, Phys. Rev. E57, 3886 (1998).

[7] R. Franzosi, L. Casetti, L. Spinelli and M. Pettini, Phys. Rev. E60, R5009 (1999).

[8] L. Casetti, E. G. D. Cohen and M. Pettini, Phys. Rev. Lett. 82, 4160 (1999).

[9] M. Nakahara “Geometry, Topology and Physics” (Hilger, Bristol, 1990).

[10] R. Franzosi, M. Pettini and L. Spinelli, Phys. Rev. Lett. 84, 2774 (2000).

[11] L. Casetti, E. G. D. Cohen and M. Pettini, Phys. Rev. E65, 036112 (2002).

[12] L. Angelani, L. Casetti, M. Pettini, G. Ruocco and F. Zamponi, Europhys. Lett. 62, 775 (2003).

[13] F. Zamponi, L. Angelani, L. F. Cugliandolo, J. Kurchan and G. Ruocco, J. Phys. A36, 8565 (2003).

[14] W. Götze in “Liquids, Freezing and the Glass transition”, eds. J. P. Hansen, D. Levesques and J. Zinn-Justin (North-Holland, Amsterdam, 1991); R. Schilling in “Disorder Effects on Relaxational Processes”, eds. R. Richert and A. Blumen (Springer-Verlag, Berlin, 1994).

[15] L. Angelani, R. di Leonardo, G. Ruocco, A. Scala and F. Sciortino, Phys. Rev. Lett. 85, 5356 (2000).

[16] K. Broderix, K. K. Bhattacharya, A. Cavagna, A. Zippelius and I. Giardina, Phys. Rev. Lett. 85, 5360 (2000).

[17] J. P. K. Doyle and D. J. Wales, J. Chem. Phys. 116, 3777 (2002).

[18] L. Angelani, R. Di Leonardo, G. Ruocco, A. Scala and F. Sciortino, J. Chem. Phys. 116, 10297 (2002).

[19] L. Angelani, G. Ruocco, M. Sampoli and F. Sciortino, J. Chem. Phys. 119, 2120 (2003).

[20] B. Doliwa and A. Heuer, Phys. Rev. E 63, 031506 (2003).

[21] E. La Nave, H. E. Stanley, and F. Sciortino, Phys. Rev. Lett. 88, 035501 (2002).

[22] A. Cavagna, I. Giardina, and G. Parisi, Phys. Rev. B 87, 11251 (1998).

[23] A. D. Bruce and R. A. Cowley, Adv. Phys. 29, 1, 111, 219 (1980).

[24] A. A. Ovchinnikov and V. A. Onischyk, Physica A167, 756 (1990).

[25] Ref. 27 has studied $H = 0$, only. But it is straightforward to generalize those results to $H \neq 0$.

[26] That the stationary points for $H = 0$ are uniquely determined by $\{\alpha_{\sigma}\}$ has been rigorously proven in Ref. 28 for $\alpha_0 = 0$, only. But the numerical solution of Eq. (20) for $\alpha_0 \neq 0$ and $H \neq 0$ has always led to a unique solution $H_{0\sigma}(\alpha_0, H)$. Therefore we will assume that $\{\alpha_{\sigma}\}$ is in a one-to-one correspondence with all stationary states as long as Eq. (22) is fulfilled.

[27] R. Franzosi and M. Pettini, Phys. Rev. Lett. 92, 060601 (2004).

[28] A. Andronico, L. Angelani, G. Ruocco, F. Zamponi, eprint cond-mat/0405188.