Energy landscape properties studied by symbolic sequences

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We investigate a classical lattice system with \( N \) particles. The potential energy \( V \) of the scalar displacements is chosen as a \( \phi^4 \) on-site potential plus interactions. Its stationary points are solutions of a coupled set of nonlinear equations. Starting with Aubry’s anti-continuum limit it is easy to establish a one-to-one correspondence between the stationary points of \( V \) and symbolic sequences \( \sigma = (\sigma_1, \ldots, \sigma_N) \) with \( \sigma_n = \pm, 0, - \). We prove that this correspondence remains valid for interactions with a coupling constant \( \epsilon \) below a critical value \( \epsilon_c \) and that it allows the use of a "thermodynamic" formalism to calculate statistical properties of the so-called “energy landscape” of \( V \). This offers an explanation why topological quantities of \( V \) may become singular, like in phase transitions. Particularly, we find the saddle index distribution is maximum at a saddle index \( v_{gs} \) as function of average energy \( \bar{v} \). Furthermore there exists an interval \( (v_{gs}^-, v_{gs}^+) \) in which the saddle index \( n_s \), as function of average energy \( \bar{v} \), is analytical in \( \bar{v} \) and it vanishes at \( v^* \), above the ground state energy \( v_g \). It can exhibit a singularity at a critical energy \( v_c \) and it vanishes at \( v_{gs}^+ \). Close to \( v_{gs} \), \( n_s(v) \) exhibits power law behavior which even holds for noninteracting particles.

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I. INTRODUCTION

We consider a classical \( N \)-particle system in three dimensions with potential energy \( V(\vec{x}_1, \ldots, \vec{x}_N) \). Both the Newtonian dynamics and the thermodynamical behavior is obtained from the knowledge of the function \( V \). Therefore one may ask: What are the characteristic features of \( V \) which are crucial for the dynamics and thermodynamics of the \( N \)-particle system? From a mathematical point of view the stationary points, in case of non-degeneracy also called critical or Morse points, yield important information on \( V \). These points are solutions of the set of coupled, nonlinear equations:

\[
\frac{\partial V}{\partial \vec{x}_n}(\vec{x}_1, \ldots, \vec{x}_N) = 0 \quad n = 1, \ldots, N .
\]

These solutions are denoted by \( \vec{x}^{(a)} = (\vec{x}_1^{(a)}, \ldots, \vec{x}_N^{(a)}) \), \( a = 1, 2, \ldots, M_N \), where \( M_N \) is believed to be exponentially in \( N \). Here some comments are in order. First, if the system is homogeneous and isotropic any translation, rotation and reflection of \( \{\{\vec{x}_n^{(a)}\}\} \) is a stationary point as well, with the same potential energy. Accordingly there is a continuous degeneracy of \( \{\{\vec{x}_n^{(a)}\}\} \). Choosing the variables \( \vec{x}_n \), e.g. with respect to the center of mass and fixing the orientation one gets rid of this degeneracy. This is assumed in the following. Second, if \( V \) is harmonic, i.e.

\[
V(\vec{x}_1, \ldots, \vec{x}_N) = \frac{1}{2} \sum_{n,m=1}^{N} \sum_{i,j=1}^{3} M_{nm}^{ij} x_n^i x_m^j .
\]

Eq. (1) becomes a set of linear equations:

\[
\sum_{m=1}^{N} \sum_{j=1}^{3} M_{nm}^{ij} x_m^j = 0 , \quad n = 1, \ldots, N; \quad i = 1, 2, 3
\]

In the generic case where \( \det(M_{nm}^{ij}) \neq 0 \), there is one solution, \( \vec{x}_n = 0 \), only. Consequently, a necessary condition for exponentially many solutions is the nonlinearity of Eq. (1). Having found all stationary points they can be characterized by their saddle index \( n_s(\vec{x}^{(a)}) = N_s(\vec{x}^{(a)})/(3N) \). \( N_s(\vec{x}^{(a)}) \) is the number of unstable directions, i.e. the number of negative eigenvalues of the Hessian \( ((\partial^2 V/\partial x_n^i \partial x_m^j)(\vec{x}^{(a)}) \). Therefore \( n_s \) varies between zero and one.

The role of \( n_s \) for the dynamics is obvious. If the trajectory \( \vec{x}(t) \) in configuration space is mostly close to stationary points with \( n_s \) very close to zero, i.e. \( \vec{x}(t) \) is close to local minima of \( V(\vec{x}_1, \ldots, \vec{x}_N) \), then the motion will mainly be...
due to thermal activation, i.e. hopping-like. In contrast, if \( \mathbf{x}(t) \) is mostly close to stationary points with \( n_s \) almost equal to one, a diffusive-like dynamics may occur. Recent MD-simulations for liquids have determined the average saddle index \( \bar{n}_s \) as function of temperature \( T \) and as function of the potential energy \( v \) per particle. It has been found that \( \bar{n}_s \) decreases with decreasing temperature and energy and its extrapolation vanishes at a temperature \( T^* \) and an energy \( v^* \), respectively. It is interesting that \( T^* \) is very close to the mode coupling glass transition temperature \( T_c \), at which a transition from ergodic to nonergodic dynamics takes place. This finding corresponds to the change from diffusive- to hopping-like motion, when decreasing the saddle index from one to zero.

There is evidence that the saddle index also plays a role for equilibrium phase transitions. For smooth, finite range and confining potentials \( V \) it has been proven that a *necessary* condition for an equilibrium phase transition is a singular change of the topology of the manifold

\[
\mathcal{M}_N(v) = \{ (\vec{x}_1, \ldots, \vec{x}_N) | V(\vec{x}_1, \ldots, \vec{x}_N) \leq v \}.
\]  

particularly, if \( M_N(v, n_s) \) is the number of stationary points of \( \mathcal{M}_N(v) \) with saddle index \( n_s \), the Euler characteristic

\[
\chi(v) = \sum_{N_s=0}^{3N} (-1)^{N_s} M_N(v, N_s/3N)
\]  

can be singular at a critical energy \( v_c \). However, for nonconfining potentials the unattainability of a purely topological criterion for the existence of equilibrium phase transition has been claimed. Besides these interesting results it has been found for a two-dimensional \( \phi^4 \)-model from numerical computations, for the exactly solvable mean-field \( XY \) model and mean-field \( k \)-trigonometric model that \( v_c \) coincides with \( N^{-1}\langle V \rangle(T_c) \), the *canonical* average of the potential energy per particle at the phase transition point \( T_c \). However, for a mean-field \( \phi^4 \)-model it has been shown that \( v_c \neq N^{-1}\langle V \rangle(T_c) \).

Finally we want to mention an interesting result for the saddle index distribution function \( P_N(n_s) \). For a binary Lennard-Jones system with up to \( N = 13 \) particles there is strong evidence that \( P_N(n_s) \) is Gaussian with a maximum at \( n_{s,max}^N \approx 1/3 \). However, the relevance of this result for dynamics and thermodynamics is not yet clear.

This exposition so far has demonstrated that the potential energy surface (PES) characterized by stationary points and their saddle indices is of physical importance. For further applications of the energy landscape description the reader may consult the textbook by D. J. Wales.

It is the motivation of the present paper to derive a relationship between \( \chi^{(\alpha)} \) and symbolic sequences \( \sigma = (\sigma_1, \ldots, \sigma_N) \) where \( \sigma_n \) takes values from an “alphabet”. This will be explained in the next section. Particularly the usefulness of this relationship for the calculation of statistical properties of the PES will be shown. To make this relation more explicit we will investigate in the 3. section noninteracting particles in an on-site potential. In the 4. section it will be explored how the features of the PES change under switching on an interaction between the particles. The final section contains a discussion of the results and some conclusions.

II. DESCRIPTION BY SYMBOLIC SEQUENCES

For some nonlinear dynamical systems it has been proven (see e.g. Refs. 12,13) that there is a one-to-one correspondence between the orbits and symbolic sequences. Therefore, the brilliant observation by Aubry that Eq. (\ref{eq:1}) for the one-dimensional Frenkel-Kontorova model is identical to the standard map, already provides a link between stationary points and symbolic sequences. This link exists for a certain class of one-dimensional models. But we think that this relationship may be more general. Let us choose a simple potential with two degrees of freedom:

\[
V(x_1, x_2) = \sin x_1 \sin x_2
\]  

Its stationary points form a square lattice with lattice constant \( \pi/2 \). The question arises how to label these stationary points. The first guess is to count the points as shown in Fig. 1.

However, there is a drawback since two neighboring points do not possess “neighboring” labels (see e.g. the points with labels 28 and 53). In order that the labelling preserves the local arrangement of the points one has to choose an “alphabet”, which are the integer numbers \( \sigma_n \in \mathbb{Z} \). Then the “sequences” \( (\sigma_1, \sigma_2, \ldots, \sigma_N) \) provide a labelling for which the local properties are preserved (cf. Figure 1a+b). Similarly, the counting of the stationary points of an arbitrary PES by \( \alpha = 1, 2, \ldots, M_N \), as done in the 1. section, is not compatible with the local properties of these points. Although the explicit determination of an “alphabet” \( A \) and of the one-to-one correspondence between the stationary points of an arbitrary PES and symbolic sequences \( (\sigma_1, \ldots, \sigma_N) \) with \( \sigma_n \in A \) in general is not possible we believe, however, that such a relationship may exist for certain potential functions \( V \). This will be proven in the third and fourth section for a certain class of functions \( V(\vec{x}_1, \ldots, \vec{x}_N) \). Of course, for a finite system there will be a finite number of
stationary points which can be labelled by \( \alpha = 1, 2, 3, \ldots \). But similarly to the simple model this will be not the appropriate labelling.

Thus, let us assume that we have found \( A \) and the one-to-one mapping:

\[
\sigma = (\sigma_1, \ldots, \sigma_N) \mapsto (\vec{x}_1(\sigma), \ldots, \vec{x}_N(\sigma)) = \mathbf{x}(\sigma)
\]

between the symbolic sequences \( \sigma \) and the stationary points \( \mathbf{x}(\sigma) \). Their potential energy is given by:

\[
E(\sigma) = V(\mathbf{x}(\sigma)).
\]

Note that depending on the specific potential energy \( V \) the sequence may contain more than \( N \) symbols, e.g. \( \sigma = (\sigma_1, \ldots, \sigma_{3N}) \). The Hessian at these stationary points is a function of \( \sigma \), too. Therefore its number of negative eigenvalues, \( N_s(\sigma) \), and accordingly the saddle index \( n_s(\sigma) \) is a function of \( \sigma \), only:

\[
n_s(\sigma) = N_s(\sigma)/(3N).
\]

In the remainder of this section we will demonstrate the usefulness of the mapping for the calculation of some properties of the PES. One of the most interesting quantities is the joint probability density \( P_N(v, n_s) \) of stationary points with potential energy \( v \) per particle and saddle index \( n_s \). Without making use of relation it can be represented as follows:

\[
P_N(v, n_s) = M_N^{-1} \int \prod_{n=1}^{N} d^3x \delta (\partial V(x)) \delta (Nv - E(\sigma)) \delta (Nn_s - N_s(\sigma))(\mathbf{x}(\sigma))
\]

One of the main technical problems for the evaluation of \( P_N(v, n_s) \) from Eq. is the occurrence of the modulus of the determinant of the Hessian. This modulus prevents the use of an integral representation by Grassmann variables. For mean-field spin glass models it has been shown that the modulus can be neglected, at least for low energies.

Now, making use of Eqs. \( \# \) and \( \# \), this probability density can also be represented by:

\[
P_N(v, n_s) = N^2 M_N^{-1} \sum_\sigma \delta (Nv - E(\sigma)) \delta (Nn_s - N_s(\sigma))
\]

which is rewritten as follows:

\[
P_N(v, n_s) = \frac{N^2 M_N^{-1}}{(2\pi)^2} \int_{-\infty}^{\infty} d\lambda \int_{-\infty}^{\infty} d\mu e^{iN[\lambda v + \mu n_s - f(\lambda, \mu)]}
\]
with the “free energy” per particle

\[ f(\lambda, \mu) = iN^{-1} \ln Z(\lambda, \mu; N) \] (13)

and the “canonical partition function”

\[ Z(\lambda, \mu; N) = \sum_{\sigma} \exp[-i(\lambda E(\sigma) + \mu N_s(\sigma))]. \] (14)

This demonstrates that, e.g. \( P_N(v, n_s) \) can be obtained from a “canonical ensemble” with probability density:

\[ \rho(\sigma) = \frac{1}{Z} e^{-i(\lambda E(\sigma) + \mu N_s(\sigma))}. \] (15)

\( \lambda \) can be interpreted as an inverse “temperature” and \( \mu \) as a “field” acting as a bias on the number of negative eigenvalues of the Hessian.

In the thermodynamic limit \( N \to \infty \) the saddle point solutions \( \lambda^*(v, n_s), \mu^*(v, n_s) \) of

\[ v = \frac{\partial f}{\partial \lambda}(\lambda, \mu), \quad n_s = \frac{\partial f}{\partial \mu}(\lambda, \mu) \] (16)

yield up to a normalization constant:

\[ P_N(v, n_s) \sim e^{Ns_0(v, n_s)} \] (17)

with the configurational entropy (per particle) of stationary points with energy per particle \( v \) and saddle index \( n_s \):

\[ s(v, n_s) = i\{\lambda^*(v, n_s)v + \mu^*(v, n_s)n_s - f(\lambda^*(v, n_s), \mu^*(v, n_s))\}. \] (18)

\( s(v, n_s) \) allows the calculation of the saddle index as function of energy. However, there are two possibilities. First, we determine the maximum \( \bar{v} \) of \( s(v, n_s) \) for \( n_s \) fixed. This yields the saddle index \( n_s(\bar{v}) \) as function of the average energy. Second, keeping the energy \( v \) fixed the maximum of \( s(v, n_s) \) yields the average saddle index \( \bar{n}_s(v) \) as function of energy. These two functions, \( n_s \) and \( \bar{n}_s \) are not identical, in general. From (18) we find:

\[ \lambda^*(\bar{v}, n_s(\bar{v})) = 0, \quad \mu^*(v, \bar{n}_s(v)) = 0 \] (19)

where Eq. (16) has been applied.

The saddle index distribution \( P_N(n_s) = \int_{-\infty}^{\infty} dv P_N(v, n_s) \) can be represented as:

\[ P_N(n_s) = \frac{NM_N^{-1}}{2\pi} \int_{-\infty}^{\infty} d\mu e^{IN[\mu n_s - f_0(\mu)]} \] (20)

with

\[ f_0(\mu) = f(0, \mu). \] (21)

For \( N \to \infty \) the saddle point solution \( \mu^*_0(n_s) \) of

\[ n_s = \frac{df_0}{d\mu}(\mu) \] (22)

leads to

\[ P_N(n_s) \sim e^{Ns_0(n_s)} \] (23)

with

\[ s_0(n_s) = i\{\mu^*_0(n_s)n_s - f_0(\mu^*_0(n_s))\}. \] (24)
Its maximum position \( n_{s}^{\text{max}} \) is given by:

\[
\mu_{0}^{*}(n_{s}^{\text{max}}) = 0.
\]  

(25)

This last paragraph has demonstrated the usefulness of the “thermodynamic” formalism based on a canonical ensemble \((15)\) in the space of symbolic sequences. This fact also allows to understand why there can be a singular topological change, e.g. as a function of \( v \). There is a lower critical dimension \( d_{\text{low}} \) such that there is a critical “temperature” \( \lambda_{-}^{-1} \) for \( d > d_{\text{low}} \) at which \( f(\lambda, \mu) \) is singular. This singularity then also occurs in the “Legendre transform” \( s(v, n_s) \) of \( f(\lambda, \mu) \).

In the third and fourth section we will show that this “thermodynamic” formalism applied to a certain class of lattice models allows an analytical calculation of \( P_{N}(v, n_s) \) from which the saddle index distribution and the energy dependence of the saddle index can be derived.

### III. NONINTERACTING PARTICLES

We consider a crystal with \( N \) lattice sites. Let \( x_n \) be the scalar displacement of particle \( n \) from its lattice site with lattice vector \( \vec{R}_n \). Then we describe the potential energy by a \( \phi^4 \)-model:

\[
V(x) = \sum_{n=1}^{N} V_0(x_n) + \epsilon V_1(x), \quad \epsilon > 0
\]  

(26)

with the double-well-like on-site potential:

\[
V_0(x) = -hx - \frac{1}{2}x^2 + \frac{1}{4}x^4, \quad h > 0
\]  

(27)

and interaction \( V_1(x) \). Choosing an appropriate energy and length scale any general quartic on-site potential can be put into the form of Eq. (27).

Inspired by Aubry’s anti-continuum limit (originally called anti-integrable limit\(^{17,18}\)) we start with \( \epsilon = 0 \), i.e. neglecting the interaction. Then Eq. (1) becomes:

\[
x_n^3 - x_n = h.
\]  

(28)

If \( h < h_c = 2/(3\sqrt{3}) \) there are three different real roots \( x_n = x_{\sigma_n}(h) \), \( \sigma_n = +, 0, - \). Therefore the stationary points are given by

\[
x_0(\sigma) = (x_{\sigma_1}, \ldots, x_{\sigma_N}),
\]  

(29)

i.e. we have found the one-to-one correspondence between stationary points and symbolic sequences with an “alphabet” \( A = +, 0, - \). Using Eqs. (8), (27) and (29) we find for the energy of the stationary points

\[
E_0(\sigma) = \sum_{n=1}^{N} [e_0 + e_1 \sigma_n + e_2 \sigma_n^2]
\]  

(30)

with

\[
e_0 = v_0, \quad e_1 = \frac{1}{2}(v_+ - v_0), \quad e_2 = -v_0 + \frac{1}{2}(v_+ + v_-)
\]  

(31)

\[
v_{\sigma} = V_0(x_{\sigma}).
\]  

These results are obvious, since the stationary points of \( V \) for \( \epsilon = 0 \) are uniquely determined by the stationary points of the local potential \( V_0(x) \). The number of extrema of \( V_0(x) \) determine the “alphabet” \( A \) and their energy \( V_0(x_{\sigma}) \) yields the coefficients \( e_\nu, \nu = 0, 1, 2 \) of \( E_0(\sigma) \). Furthermore the function \( N_s(\sigma) \) is also easily determined. Since we identify the maximum of \( V_0(x_n) \) with \( \sigma_n = 0 \), its absolute and local minimum, respectively, with \( \sigma_n = + \) and \( \sigma_n = - \), it is:

\[
N_s(\sigma) = \sum_{n=1}^{N} (1 - \sigma_n^2).
\]  

(32)
Having found the “alphabet” \( \mathcal{A} \), the mapping \( \mathcal{S} \) as well as \( E_{\mathcal{S}}(\sigma) \) and \( N_{\mathcal{S}}(\sigma) \) we can calculate \( P_N(v, n_s) \) as described in the previous section. The calculation of the “partition function” \( \mathcal{Z} \) is easy. One gets from Eq. (33):

\[
f(\lambda, \mu) = (\lambda e_0 + \mu) + i \ln [1 + 2e^{-i(\lambda e_2 - \mu)} \cos \lambda e_1].
\]  

(33)

The saddle point solutions of Eq (16) are easily determined leading to \( P_N(v, n_s) \) from Eq. (17) with:

\[
s(v, n_s) = -[n_-(v, n_s) \ln n_-(v, n_s) + n_+(v, n_s) \ln n_+(v, n_s) + n_s \ln n_s]
\]

(34)

where:

\[
n_\pm(v, n_s) = \pm(v_+ - v_+)^{-1}[(v_+ - v) + (v_0 - v_+)n_s].
\]

(35)

for asymmetric double well, i.e. \( v_+ \neq v_- \). Quite analogously one finds the saddle point \( \mu^*_0(n_s) \):

\[
\mu^*_0(n_s) = i \ln \frac{1 - n_s}{2n_s}
\]

(36)

leading to:

\[
s_0(n_s) = -[n_s \ln n_s + (1 - n_s) \ln(1 - n_s)/2]
\]

(37)

for symmetric and asymmetric double well potentials.

To determine the relation between the saddle index and energy for symmetric double well, i.e., for \( h = 0 \), we have to realize that \( n_s \) and \( v \) are no longer independent variables. This can easily be seen from Eq. (31), taking \( c_1 = 0 \) into account, which follows from Eq. (31). Then we arrive at

\[
E(\sigma) = Nv_+ + (v_0 - v_+)N_s(\sigma)
\]

(38)

where Eqs. (31) and (32) were used. This yields immediately:

\[
v(n_s) = v_+ + (v_0 - v_+)n_s,
\]

(39)

and no distinction between \( n_s(\tilde{v}) \) and \( \tilde{n}_s(v) \) exists. Because of the dependence of both variables \( v \) and \( n_s \) on each other their joint probability density reduces to \( P_N(n_s) \) which is proportional to the probability density of \( v \). From Eqs. (30) and (31) we find for symmetric and asymmetric double wells:

\[
n_s^{\text{max}} = 1/3
\]

(40)

which is the maximum of \( s_0(n_s) \) (Eq. (37)) and therefore the maximum of the saddle index distribution \( P_N(n_s) \). \( P_N(n_s) \) is a Gaussian for \( |n_s - n_s^{\text{max}}| = O(1/\sqrt{N}) \), in agreement with the numerical result for Lennard-Jones clusters.

Let us return to the asymmetric double well. The functions \( n_s(\tilde{v}) \) and \( \tilde{n}_s(v) \) can be obtained from the maximum of \( s(v, n_s) \) for fixed \( n_s \) and fixed \( v \), respectively. As a result we get

\[
n_s(\tilde{v}) = \frac{(v_- + v_+) - 2\tilde{v}}{-2v_0 + (v_- + v_+)}
\]

(41)

and

\[
[n_+(v, \tilde{n}_s)]^{\tilde{n}_s - v_+} = \left[\frac{n_-(v, \tilde{n}_s)}{n_s}\right]\frac{\tilde{n}_s - v_-}{v_- - v_+}
\]

(42)

with \( v_-, v_0, v_+ \) from Eq. (31) and \( n_+(v, \tilde{n}_s) \) from Eq. (35). \( n_s \) is a linear function of the average energy \( \tilde{v} \). It vanishes at \( \tilde{v}^* = \frac{1}{2}(v_- + v_+) \) which is above the ground state energy \( v_\text{gs} = v_- \), since we assumed asymmetric double wells. \( n_s \) becomes one for \( \tilde{v} = v_0 \), the height of the unstable extremum of \( V_0(x) \). \( n_s(\tilde{v}) \) is presented in Figure 2a. Eq. (12) is an implicit one for \( \tilde{n}_s(\tilde{v}) \), which can not be solved analytically. The numerical result is shown in Figure 2b. There are two features to be mentioned. First, \( \tilde{n}_s(\tilde{v}) \) vanishes at the ground state energy \( v_\text{gs} = v_+, \) only. Second, it can be proven analytically that it exhibits a power law behavior in \( v \) close to \( v_\text{gs} \) (cf. the inset of Fig. 2b):

\[
\tilde{n}_s(\tilde{v}) \approx \left(\frac{v - v_\text{gs}}{v_- - v_\text{gs}}\right)^{\delta_0} + O((\frac{v - v_\text{gs}}{v_- - v_\text{gs}})^{\delta_0+1}) + O((\frac{v - v_\text{gs}}{v_- - v_\text{gs}})^{2\delta_0-1})
\]

(43)
FIG. 2: (a) saddle index $n_s$ as function of the average energy $\bar{v}$, (b) average saddle index $\bar{n}_s$ as function of the energy $v$. Both figures are for noninteracting particles ($\epsilon = 0$) with $v_0 = 0$, $v_- = -1$ and $v_+ = -1.8$. The inset in Fig. 2b shows the comparison of the exact result for $\bar{n}_s(v)$ from Eq. 42 (solid line) with the leading power law from Eq. 43 (dashed line).

It is interesting that we find for $\bar{n}_s(v)$ (in contrast to $n_s(\bar{v})$) a nonanalytical $v$-dependence close to $v_{gs}$, despite the neglection of interactions. In the next section we will show that this power law also exists in case of interactions.

So far we have demonstrated that the “thermodynamic” formalism can be applied to get the saddle index distribution, $n_s(\bar{v})$ and $\bar{n}_s(v)$. $n_s(\bar{v})$ and $\bar{n}_s(v)$ also follow directly from the saddle points $\lambda^*$ and $\mu^*$ (cf. Eq. 19). This has not been used, because $\lambda^*(v, n_s)$ is a rather lengthy expression. The results 47, 48 concerning the saddle index distribution, and 49 for $n_s(\bar{v})$ can be obtained much easier as follows. The number of stationary points characterized

for $\frac{v}{v_{gs}} - 1 \ll 1$ with an exponent:

$$\delta_0 = \frac{v_0 - v_+}{v_- - v_+} > 1 .$$

(44)
by $N_\sigma$, which is the number of $\sigma_n$ of $\sigma$ equal to $\sigma \in \{-,0,+,\}$, is given by

$$\frac{N!}{N_+!N_0!N_-!}$$

(45)

which for fixed saddle index $n_s = N_0/N$ has its maximum weight for $N_+ = N_- = \frac{1}{2}(N - N_s)$. Substituting this into expression (45) we get by use of Stirling’s formula:

$$P_N(n_s) \sim e^{N_s n_s}$$

(46)

with $s_0(n_s)$ from Eq. 57. The maximum position $n_s^{max}$ is also obvious. If $N_s^{max} = N_0^{max} = N_0^{max} = N/3$, expression (45) takes its maximum value. Therefore $n_s^{max} = N_0^{max}/N = 1/2$.

Next we use $\overline{v}(n_s)$ from Eq. (37). The maximum position $n_s^{max}$ is also obvious. If $N_s^{max} + N_s^{max} = N_0^{max} \equiv N_s^{max} - N_s^{max} \equiv N/3$, expression (45) takes its maximum value. Therefore $n_s^{max} = N_0^{max}/N = 1/3$.

Next we use $\overline{v}(n_s)$ from Eq. (30) to calculate $\overline{v}(n_s) = 1/2(v_+ + v_-) + [v_0 - 1/2(v_+ + v_-)]n_s$

(48)

from which Eq. (41) is reproduced. The question arises: Which of these features remain valid in the presence of interactions? This will be discussed in the next section.

IV. INTERACTING PARTICLES

Now we will study the influence of interactions on the results derived in the previous section. $V(x)$ is given by Eq. (20) and (27) where we will assume that the interaction energy $V_1(x)$ is (i) at least twice differentiable and (ii) does not grow faster than quartic. To investigate the labelling of all stationary points of $V(x)$ for $\epsilon > 0$ we adopt the method used by MacKay and Aubry and MacKay and Sepulchre to prove the existence of breathers, and to investigate multistability in networks, respectively, i.e. the implicit function theorem. In the last section we have proven for $\epsilon = 0$ that all stationary points $x_0(\sigma) \equiv x(\epsilon = 0, \sigma)$ are uniquely labelled by symbolic sequences $\sigma$, $\sigma_n = +,0,-$, provided $h < h_c$. The eigenvalues $\lambda_\nu(0, \sigma)$ of the Hessian ($\epsilon = 0$) are nonzero for all $\sigma$ and $h < h_c$ with:

$$\text{sign } \lambda_\nu(0, \sigma) = -1 + 2\sigma_n^2$$

(49)

This implies that

$$\det(\frac{\partial^2 V}{\partial x_n \partial x_m}(x_0(\sigma))) \neq 0$$

(50)

for all $\sigma$. Let us introduce the functions

$$\phi_n(\epsilon, x) = \frac{\partial V}{\partial x_n}(\epsilon, x),$$

(51)

which are at least one times differentiable. Note that we have made the $\epsilon$-dependence of $V$ explicit. Then Eq. 11 reads:

$$\phi_n(\epsilon, x) = 0, \quad n = 1, \ldots, N.$$

(52)

We have found solutions $x_0(\sigma)$ for $\epsilon = 0$:

$$\phi_n(0, x_0(\sigma)) = 0, \quad n = 1, \ldots, N.$$

(53)

Because the Jacobian:

$$\frac{\partial(\phi_1, \ldots, \phi_N)}{\partial(x_1, \ldots, x_N)}(x_0(\sigma)) = \det(\frac{\partial^2 V}{\partial x_n \partial x_m}(x_0(\sigma))) \neq 0$$

(54)
for all \( \sigma \) and \( 0 \leq h < h_c \), we can apply the implicit function theorem\(^{21}\) which guarantees the existence of a neighborhood \( \bar{U}(\sigma) \) of \( (\epsilon = 0, x_0(\sigma)) \in \mathbb{R}^{N + 1} \), of an open set \( W(\sigma) = [0, \epsilon_c(\sigma)] \subset \mathbb{R} \) and of functions \( x_n(\epsilon, \sigma), n = 1, \ldots, N \) (at least one times differentiable) such that

\[
\phi_n(\epsilon, x(\epsilon, \sigma)) = 0, \tag{55}
\]

for all \( \epsilon \in W(\sigma) \) and all \( \sigma \). This leads to a nonvanishing critical value

\[
\epsilon_c = \min_{\sigma} \epsilon_c(\sigma) > 0 \tag{56}
\]

such that \( x(\epsilon, \sigma) \) are stationary points of \( V(x) \) for \( 0 \leq \epsilon < \epsilon_c \). Therefore the one-to-one correspondence between these points and symbolic sequences \( \sigma \) with \( \sigma_n \in \{+, 0, -\} \) holds for \( 0 \leq \epsilon < \epsilon_c \) and \( h < h_c \).

At \( \epsilon_c \) a bifurcation occurs at which stationary points disappear and new ones may be created. Accordingly the “alphabet” and/or the mapping between stationary points and symbolic sequences will change at \( \epsilon_c \). This bifurcation is signalled by the vanishing of at least one of the eigenvalues \( \lambda_n(\epsilon_c, \sigma) \), for one or more sequences \( \sigma \). Consequently, it is

\[
\text{sign} \lambda_n(\epsilon, \sigma) = \text{sign} \lambda_n(0, \sigma) \tag{57}
\]

for \( 0 \leq \epsilon < \epsilon_c \), since a change of sign occurs at \( \epsilon_c \), only. This has the strong implication that the saddle index of \( x(\epsilon, \sigma) \) is identical to that of \( x(0, \sigma) \), which is given by the number \( N_0 \) of \( \sigma_n = 0 \). This result can also be put into other words: Although the relative heights of the stationary points will change with \( \epsilon \), the topology will remain unchanged. By this we mean that a stationary point with \( N_0 \) unstable directions remains a stationary point with \( N_s \) unstable directions for \( 0 \leq \epsilon < \epsilon_c \). We note, that this result requires condition (ii) for the function \( V_1 \). In case that \( V_1(x) \) grows faster than quartic, additional stationary points may occur already for arbitrary small values of \( \epsilon \). Validity of (ii) guarantees that \( x(\epsilon, \sigma) \), which are continuously connected to \( x(0, \sigma) \), are the only solutions of Eq. (1).

Some general conclusions can be drawn from this result. Since the one-to-one correspondence between the stationary points and \( \sigma \) is preserved for \( 0 \leq \epsilon < \epsilon_c \), the saddle index distribution \( P_N(n_s) \) and accordingly \( n_s^{\max} = 1/N \) remains the same. Although the calculation of \( n_s(\bar{v}) \) and \( \bar{n}_s(\bar{v}) \) needs the knowledge of the energy \( E(\sigma) \) of the stationary points, one can prove some general properties of both functions without using the explicit form of \( E(\sigma) \). Let us begin with \( n_s(\bar{v}) \) which is obtained from \( \bar{v}(n_s) \). As already shown in the last section \( \bar{v}(n_s) \) is directly obtained from

\[
\bar{v}(n_s) = (NM_N(n_s))^{-1} \sum_{N_s(\sigma) = n_s} E(\sigma) \tag{58}
\]

where \( M_N(n_s) \) is the number of \( \sigma \) with \( N_s(\sigma) = n_s N \). \( n_s = 0 \) yields all local minima of \( V(x) \), including the ground state. Most of these minima have an energy above the ground state energy \( N v_{gs} \), i.e. it is:

\[
\bar{v}(0) > (NM_N)^{-1} N v_{gs} M_N(n_s) = v_{gs}. \tag{59}
\]

For \( n_s = 1 \), i.e. \( N = N_s \), there is only one stationary point, the maximum of \( V(x) \), with energy \( E(0, \ldots, 0) \) such that

\[
\bar{v}(1) = N^{-1} E(0, \ldots, 0) = v_{\max}. \tag{60}
\]

From this we find that \( n_s(\bar{v}) \) vanishes at \( \bar{v}^* > v_{gs} \) and becomes one at \( \bar{v} = v_{\max} \). Whether or not \( n_s(\bar{v}) \) is always monotonically increasing with increasing \( \bar{v} \) is not clear. In contrast to \( n_s(\bar{v}) \), the average saddle index \( \bar{n}_s(\bar{v}) \) is nonzero for all \( v > v_{gs} \). Without presenting a rigorous prove, let us explain why this should be true. The ground state belongs to \( n_s = 0 \) and is characterized by \( \sigma \) with \( \sigma_{gs}^{\text{max}} = + \) or \( - \). This also holds, if it is degenerate. Now, let us choose \( K \) particles \( j_1, \ldots, j_K \) for which we change \( \sigma_{j_k} \in \{+, -\} \) into \( \sigma_{j_k} = 0 \). The corresponding stationary point has \( n_s = K/N \). If \( K = 1 \), we generate a “defect” with excitation energy \( \epsilon_{j_1} \). Then \( K \) “defects” have an energy

\[
E_{j_1 \ldots j_K} = N v_{gs} + \sum_{k=1}^{K} \epsilon_{j_k} + (\ldots), \text{ where } (\ldots) \text{ is the interaction energy of the defects. It is obvious that } E_{j_1 \ldots j_K}/N \to v_{gs}
\]

for \( K \to \infty, N \to \infty \) with \( K/N \to 0 \). “Defect” configurations with fixed energy \( v = E_{j_1 \ldots j_K}/N \) will have fluctuating \( K \) with \( 0 < K/N \). If we choose \( v - v_{gs} \) arbitrary small but nonzero the average saddle index \( \bar{n}_s = K/N \) will be small, but finite, too. Consequently \( \bar{n}_s \) can only vanish at \( v_{gs} \). Since there is one stationary point (maximum) with energy \( v_{\max} \), only, it must be \( \bar{n}_s(v_{\max}) = 1 \), i.e.

\[
n_s(\bar{v} = v_{\max}) = \bar{n}_s(v_{\max}) = 1. \tag{61}
\]

Again, it is not obvious whether \( \bar{n}_s(\bar{v}) \) is monotonously increasing with increasing \( v \).
To get more quantitative results for \( n_s(\bar{v}) \) and \( \bar{n}_s(v) \), we have to specify \( E(\sigma) \). Since the solutions \( x(\epsilon, \sigma) \) are not known exactly this can only be done approximately. In the following we will present the crucial steps leaving out technical details. Our purpose is to derive the qualitative structure of \( E(\sigma) \). To be explicit we choose harmonic interactions:

\[
V_1(x) = \frac{1}{2} \sum_{n,m} V_{nm} x_n x_m, \quad V_{nn} = 0. \tag{62}
\]

with coupling coefficients \( V_{nm} = V(\bar{R}_n - \bar{R}_m) \). Using \( V_1(x) \) from Eq. (62), Eq. (11) takes the form:

\[
-x_n + x_n^3 - h = -\epsilon \sum_m V_{nm} x_m \tag{63}
\]

which can be solved by iterations:

\[
-x_n^{(1)} + (x_n^{(1)})^3 - h = -\epsilon \sum_m V_{nm} x_m^{(0)}, \quad x_m^{(0)} = x_m(\epsilon = 0, h) = x_{\sigma_m}(h) \tag{64}
\]

etc. We remind the reader that \( x_{\sigma_m}(h) \) are the roots of Eq. (28). If \(|h - \epsilon \sum_{m} V_{nm} x_{\sigma_m}(h)| < h_c \) for all \( \sigma \), Eq. (34) has three real roots:

\[
x_{n}^{(1)}(\epsilon, \sigma) = x_{\sigma_n}(h - \epsilon \sum_{m} V_{nm} x_{\sigma_m}(h)) \tag{65}
\]

which will be expanded with respect to \( \epsilon \):

\[
x_{n}^{(1)}(\epsilon, \sigma) = x_{\sigma_n}(h) - \epsilon x_{\sigma_n}'(h) \sum_{m} V_{nm} x_{\sigma_m}(h) + \frac{1}{2} \epsilon^2 x_{\sigma_n}''(h) \sum_{m,m'} V_{nm} V_{nm'} x_{\sigma_m}(h) x_{\sigma_{m'}}(h). \tag{66}
\]

\( \frac{d^p x_{\sigma_n}(h)}{dh^p} \) can be represented as follows:

\[
\frac{d^p x_{\sigma_n}(h)}{dh^p} = \sum_{i=0}^{p} x_{n}^{(i)}(h) \sigma^i \tag{67}
\]

where \( x_{i}^{(\ell)} \) is easily expressed by the \( \ell \)-th derivative of \( x_{\sigma_n}(h) \), \( \sigma = +, 0, - \). Using Eq. (67) we get from Eq. (66)

\[
x_{n}^{(1)}(\epsilon, \sigma) = \sum_{i=0}^{2} x_{i}^{(1)}(h) \sigma^i + \epsilon \sum_{i=0}^{2} x_{i,n}^{(1)}(h) \sigma^i + \frac{1}{2} \epsilon^2 \sum_{i=0}^{2} x_{i,n}^{(2)}(h) \sigma^i + \cdots \tag{68}
\]

with:

\[
 x_{i}^{(1)}(h) \equiv x_{i}^{(0)}(h), \quad x_{n,i}^{(1)}(h) = -x_{n,i}^{(0)}(h) \sum_{m} V_{nm} x_{i,m}(h), \text{ etc.} \tag{69}
\]

The substitution of \( x_{n}^{(1)}(\epsilon, \sigma) \) from Eq. (68) into \( V(x) \) with \( V_1(x) \) from Eq. (62) leads to:

\[
E_{1}(\sigma) \equiv V(x^{(1)}(\sigma)) = \sum_{n} [c_{0}^{(1)}(\epsilon) + c_{1}^{(1)}(\epsilon) \sigma_n + c_{2}^{(1)}(\epsilon) \sigma_n^2] + \epsilon \sum_{n_1 \neq n_2} [A_{n_1 n_2}^{(1)}(\sigma_n^2 \sigma_n^2 + \sigma_n \sigma_n^2 + \sigma_n^2 \sigma_n^2) + B_{n_1 n_2}^{(1)}(\sigma_n^2 \sigma_n^2 + \sigma_n \sigma_n^2 + \sigma_n^2 \sigma_n^2) + C_{n_1 n_2}^{(1)}(\sigma_n^2 \sigma_n^2 + \sigma_n \sigma_n^2 + \sigma_n^2 \sigma_n^2) + D_{n_1 n_2}^{(1)}(\sigma_n^2 \sigma_n^2 + \sigma_n \sigma_n^2 + \sigma_n^2 \sigma_n^2) + \cdots] \tag{70}
\]
where \( (\cdots) \) are four-, five- etc. body interactions which are of order \( \epsilon^3, \epsilon^4 \) etc. The coefficients in capital letters in Eq. (70) can be expressed by \( x_{i_n}(h) \), \( x_{n, i_n, i_m}(h) \), etc., \( h \) and \( V_{nm} \). \( E^{(3)}(\sigma) \) is a kind of generalized Blume-Emery-Griffiths model. Using higher order iterates the corresponding energy \( E^{(\nu)}(\sigma) \) will be similar to Eq. (70) with “renormalized” coefficients \( e_i^{(\nu)}, A^{(\nu)}_{n_1 n_2}, \) etc. On the other hand it is obvious that any function \( f(\sigma) \) can be represented by a form as given on the r.h.s. of Eq. (70). Therefore we choose for \( E(\sigma) \) the r.h.s. of Eq. (70) without the superscripts.

We begin with the calculation of \( n_s(\bar{v}) \). Taking \( \lambda^*(\bar{v}, n_s(\bar{v})) = 0 \) (cf. Eq. (16)) into account the saddle point equations (16) reduce to:

\[
\bar{v} = \frac{1}{N \cdot Z(0, \mu^*; N)} \sum_{\sigma} E(\sigma)e^{-i\mu^* N_s(\sigma)},
\]

(71)

\[
n_s = \frac{1}{N \cdot Z(0, \mu^*; N)} \sum_{\sigma} N_s(\sigma)e^{-i\mu^* N_s(\sigma)}
\]

(72)

\( \mu^*(n_s) \) is easily obtained from the second equation of (71):

\[
\mu^*(n_s) = i \ln \frac{2n_s}{1 - n_s}
\]

(73)

and the first one can be written as follows:

\[
\bar{v} = \frac{1}{N} \left( \sum_n (e_0(\epsilon) + e_1(\epsilon)(\sigma_n)_0 + e_2(\epsilon)(\sigma_n^2)_0) + \right.
\]

\[
+ \epsilon \sum_{n_1 \neq n_2} [A_{n_1 n_2}(\sigma_{n_1})_0(\sigma_{n_2})_0 + B_{n_1 n_2}(\sigma_{n_1}^2)_0(\sigma_{n_2})_0 + (\sigma_{n_1})_0(\sigma_{n_2}^2)_0) +
\]

\[
+ C_{n_1 n_2}(\sigma_{n_1}^2)_0(\sigma_{n_2}^2)_0 + \cdots]
\]

(74)

with

\[
(\kappa(\sigma))_0 = \sum_{\sigma=+0,-} f(\sigma)e^{-i\mu^* (1-\sigma^2)} / \sum_{\sigma=+0,-} e^{-i\mu^* (1-\sigma^2)}.
\]

Taking \( \mu^* \) from Eq. (72) into account one easily finds:

\[
(\sigma_n)_0 = 0 \hspace{1cm} (\sigma_n^2)_0 = 1 - n_s.
\]

(75)

This result is obvious, since for \( N_s = n_s N \) fixed the maximum weight of expression (15) is obtained for \( N_+ = N_- = N(1 - n_s)/2 \) which immediately implies Eq. (15). Introducing the result from Eq. (15) into Eq. (14) yields:

\[
\bar{v}(n_s) = e_0(\epsilon) + e_2(\epsilon)(1 - n_s) + \epsilon C_2(0)(1 - n_s)^2 + \epsilon^2 C_3(0)(1 - n_s)^3 + \cdots
\]

(76)

with:

\[
C_2(0) = \sum_{n_2 \neq 0} C_{0n_2}, \hspace{1cm} C_3(0) = \sum_{0 \neq n_2, n_3 \neq 0} C_{0n_2n_3}, \cdots
\]

(77)

where the lattice translational invariance has been taken into account. For \( \epsilon \) small enough, \( \bar{v}(n_s) \) is monotonous in \( n_s \) and we can solve Eq. (70) for \( n_s(\bar{v}) \):

\[
n_s(\bar{v}) = 1 + \frac{\bar{v} - (e_0(\epsilon) + e_2(\epsilon))}{e_2(\epsilon)} - \frac{\epsilon C_2(0)(\bar{v} - (e_0(\epsilon) + e_2(\epsilon)))^2 + 0(\epsilon^2)}{e_2(\epsilon)}.
\]

(78)

Note that the bare one-particle quantities \( e_i \) (cf. Eqs. (30), (31)) are “renormalized” to \( e_i^{(\nu)}(\epsilon) \) which depend on the coupling constants \( V_{nm} \). Putting in Eq. (78) \( \epsilon = 0 \), one recovers (by use of Eq. (31)), the result (41)). The interaction between the particles has two effects. First, it “renormalizes” the one-particle coefficients \( e_i, i = 0, 1, 2 \) such that \( e_1(\epsilon) \neq 0 \), in general. This corresponds to a non-symmetric, effective on-site potential. Second, \( n_s(\bar{v}) \) becomes nonlinear. Its curvature depends on the sign of the effective coupling constant \( C_2(0) \).

The calculation of \( \bar{n}_*,(\bar{v}) \) is much more involved, because one has to perform averages with respect to \( \exp[-i\lambda E(\sigma)] \), which contains the interactions. This is in contrast to the averaging with \( \exp[-i\mu N_s(\sigma)] \) (cf. Eq. (71)) which factorizes. Therefore an analytically exact determination of \( \bar{n}_*(\bar{v}) \) for all \( \bar{v} \) is not possible. But, in the following we
will demonstrate that the “thermodynamic” formalism can be applied to get \( \bar{n}_s(v) \) for \( v/v_{gs} - 1 \ll 1 \). In that limit we can perform a cumulant expansion. The simplest case is a “ferro-elastic” ground state, i.e. \( \sigma_n^{\mu} \equiv +, \) as for the non-interacting particles. For \( v \) close to \( v_{gs} = E(+, \ldots, +)/N \) only such stationary points exist for which a low concentration of \( \sigma_n^{\mu} \) deviate from +. Therefore we introduce “defect” variables:

\[
\tau_n = 1 - \sigma_n \quad . 
\] (79)

The ground state belongs to \( \tau_n = 0 \). \( \tau_n = 1 \) or 2 indicates a “defect”. Replacing in Eq. (85) \( \sigma_n \) by \( \tau_n \) yields:

\[
E(\tau) = E(+, \ldots, +) + E_0(\tau) + E_1(\tau) 
\] (80)

with

\[
E_0(\tau) = \sum_n [\hat{\epsilon}_1(\tau)\tau_n + \hat{\epsilon}_2(\tau)\tau_n^2] 
\] (81)

\[
E_1(\tau) = \sum_{n_1 \neq n_2} [\hat{A}_{n_1n_2}(\tau)\tau_{n_1}\tau_{n_2} + \hat{B}_{n_1n_2}(\tau)(\tau_{n_1}^2\tau_{n_2} + \tau_{n_1}\tau_{n_2}^2) + \hat{C}_{n_1n_2}(\tau)\tau_{n_1}^2\tau_{n_2}^2] + \ldots 
\]

where \( \hat{A}_{n_1n_2}, \hat{B}_{n_1n_2}, \) etc. contain different orders in \( \epsilon \) and vanish for \( \epsilon = 0 \). They can easily be expressed by \( \hat{A}_{n_1n_2}, \hat{B}_{n_1n_2}, \) etc. For \( \hat{\epsilon}_1(\tau), \hat{\epsilon}_2(\tau) \) one obtains:

\[
\hat{\epsilon}_1(\tau) + \hat{\epsilon}_2(\tau) = e_0(\tau) + e_{gs}(\tau) = e_0(\tau) + \epsilon(v_0(\tau) - v_{gs}(\tau)) 
\] (82)

\[
2(\hat{\epsilon}_1(\tau) + 2\hat{\epsilon}_2(\tau)) = e_0(\tau) + e_1(\tau) + e_2(\tau) - v_{gs}(\tau) = v(\tau) - v_{gs}(\tau) 
\]

where \( v_0(\tau) \) and \( v(\tau) \) are obtained from Eq. (81) by replacing \( \epsilon \) by \( e_\tau(\tau) \). Using a cumulant expansion we get for the “free energy”:

\[
f(\lambda, \mu) = v_{gs}\lambda + f_0(\lambda, \mu) + \lambda\frac{1}{N}(E_1(\tau))_0 + 
\]

\[
+i\lambda^2\frac{1}{2N}[(E_1(\tau)_0^2 - (E_1(\tau))^2)] + \ldots 
\]

The quantities with subscript 0 are obtained with the unperturbed “canonical ensemble”:

\[
\rho_0(\tau) = \frac{1}{Z_0} e^{-(\lambda f_0(\tau)+\mu N_s(\tau))} 
\] (84)

where \( N_s(\tau) \) is obtained from Eq. (82) by use of Eq. (79). Then the saddle point equations (16) are as follows:

\[
v - v_{gs} = \frac{\partial f_0}{\partial \lambda} + \frac{1}{N}(E_1(\tau)_0 + \lambda\frac{\partial}{\partial \lambda}(E_1(\tau)_0) + \cdots 
\] (85)

\[
n_s = \frac{\partial f_0}{\partial \mu} + \frac{1}{N}\lambda\frac{\partial}{\partial \mu}(E_1(\tau)_0) + \cdots 
\]

Here, we have only given terms up to the first cumulant. \( f_0(\lambda, \mu) \) can easily be calculated from Eq. (84). \( \frac{\partial f_0}{\partial \lambda} \) and \( \frac{\partial f_0}{\partial \mu} \) are linear in \( \langle \tau_n \rangle_0 \) and \( \langle \tau_n^2 \rangle_0 \) where:

\[
\langle \tau_n \rangle_0 = \frac{A + 2B}{1 + A + B}, \quad \langle \tau_n^2 \rangle_0 = \frac{A + 4B}{1 + A + B} 
\] (86)

with:

\[
A = \exp[-i(\lambda(\hat{\epsilon}_1 + \hat{\epsilon}_2) + \mu)], \quad B = \exp[-i2\lambda(\hat{\epsilon}_1 + 2\hat{\epsilon}_2)]. 
\] (87)

The correction terms in Eq. (85), i.e. the first, second, etc. cumulants are quadratic, cubic, etc. in \( \langle \tau_n \rangle_0 \) and \( \langle \tau_n^2 \rangle_0 \). The l.h.s. of Eq. (85) becomes arbitrary small since \( v - v_{gs} \to 0 \) implies \( n_s \to 0 \). Then it follows that \( \langle \tau_n \rangle_0 \) and \( \langle \tau_n^2 \rangle_0 \) in leading order are linear in \( v - v_{gs} \) and \( n_s \) and that the cumulant terms in Eq. (85) are of higher order. After having performed in Eq. (85) the differentiations, we are allowed to set \( \mu(v, \bar{n}_s) = 0 \), since we are calculating \( \bar{n}_s \) as function of \( v \). Writing \( A \) and \( B \) as the result for \( \epsilon = 0 \) plus a correction:

\[
A = \bar{n}_s(1 + \delta A), \quad B = \frac{(v - v_{gs}) - (\hat{\epsilon}_1 + \hat{\epsilon}_2)\bar{n}_s}{2(\hat{\epsilon}_1 + 2\hat{\epsilon}_2)}(1 + \delta B) 
\] (88)
one finds from Eq. (S5):

\[ \delta_A \simeq (a\bar{n}_s + b(v - v_{gs})) \ln \bar{n}_s, \quad \delta_B \simeq (c\bar{n}_s + d(v - v_{gs})) \ln \bar{n}_s \]  

(89)

in leading order in \( v - v_{gs} \) and \( \bar{n}_s \). The coefficients \( a, b, c, \) and \( d \) depend on \( \sum_{n_2 \neq 0} \tilde{A}_{0n_2}^{(\epsilon)}, \sum_{n_2 \neq 0} \tilde{B}_{0n_2}^{(\epsilon)}, \sum_{n_2 \neq 0} \tilde{C}_{0n_2}^{(\epsilon)}, \) etc. and vanish for \( \epsilon = 0 \). With Eqs. (S8) and (S9) we can eliminate \( \lambda \) from Eq. (S7) which finally yields:

\[ \bar{n}_s(v) \simeq x^\delta + O(x^{\delta+1} \ln x) + O(x^{2\delta-1} \ln x) \]  

(90)

with

\[ x = \frac{v - v_{gs}(\epsilon)}{v_-(\epsilon) - v_+(\epsilon)} \]  

(91)

and

\[ \delta(\epsilon) = \frac{v_0(\epsilon) - v_{gs}(\epsilon)}{v_-(\epsilon) - v_{gs}(\epsilon)} \]  

(92)

where we used Eq. (S2). Comparison of the result (90) with the corresponding one for noninteracting particles (Eq. (13)) shows that the interactions do not change the power law dependence. But, they lead to modified next-to-leading order corrections, containing logarithmic dependence on \( v - v_{gs} \).

V. DISCUSSIONS AND CONCLUSIONS

The purpose of the present paper has been twofold. First of all, we wanted to establish a relationship between the stationary points which are solutions of a set of coupled, nonlinear equations, and symbolic sequences \( \sigma \), where \( \sigma_n \) takes values from an alphabet \( A \). We have proven for the class of \( \phi^4 \)-models that such a unique relation exists, provided that the coupling parameter \( \epsilon \) is below a critical value \( \epsilon_c \). This proof is based on Aubry’s anti-continuum limit22,23 and the application of the implicit function theorem, similar to the proof of existence of breather by MacKay and Aubry17,18. Assuming that such a one-to-one correspondence exists in general we have demonstrated in the second section that one can use a “thermodynamic” formalism for the calculation of statistical properties of the stationary points. Consequently, this description allows to investigate topological quantities of the so-called “energy landscape” of a potential energy \( V(x_1, \ldots, x_n) \). Particularly, it yields an explanation why a topological singularity, e.g. for the Euler characteristic of the manifold \( M_\sigma(v) \) (cf. Eq. (1)) can occur. We stress that our “thermodynamic” formalism is not the same as that recently used to calculate the full canonical partition function22. There the configuration space has been divided into basins of the stationary points. Taking also the vibrational degrees of freedom into account these authors were able to calculate the canonical partition function, under a couple of assumptions.

The relationship between stationary points and sequences \( \sigma \) already proves that there are in total \( n_A^n = \exp(N \ln n_A) \) stationary points. \( n_A \) is the number of “letters” of the “alphabet” \( A \). For rather special models this has already been shown to be true24,25,23,24. Then it is easy to calculate the saddle index distribution function \( P_N(n_s) \) because the number of negative eigenvalues of the Hessian can be related to the number of \( \sigma_n \)’s taking certain values. For the \( \phi^4 \)-model this value is 0. Simple combinatorics leads for \( P_N(n_s) \) to a Gaussian of width proportional to \( N^{-1/2} \) and a maximum at \( n_s^{\text{max}} = 1/3 \). It is interesting that this value obtained for a \( \phi^4 \)-lattice model coincides with the result found for Lennard-Jones clusters for \( 4 \leq N \leq 92 \). Is this just an accident? The answer is not clear. It may be true that the potential energy landscape of a liquid can be decomposed into basic “units” which are double-well-like. Of course, the smallest “unit” one can choose are two adjacent local minima. Because both must be connected by a barrier one arrives at a double-well potential with extrema being labelled by \( +, 0, - \). The main open question is: Can one really construct the full energy landscape by connecting such double well potentials and accounting correctly for its connectivity?

For the \( \phi^4 \)-model we have found the energy dependence of the saddle index. It has become clear that the functions \( n_\sigma(\bar{v}) \) and \( \bar{n}_s(v) \) are not identical. Whereas both functions are equal one at the largest possible value for \( \bar{v} \) and \( v \):

\[ \bar{v}_{\text{max}} = v_{\text{max}} = N^{-1}E(0, \ldots, 0), \]  

they have different behavior below \( N^{-1}E(0, \ldots, 0) \). \( n_\sigma(\bar{v}) \) vanishes at \( \bar{v}^* \) above the ground state energy \( v_{gs} \) and \( \bar{n}_s(v) \) becomes zero at \( v = v_{gs} \), only. We think that this behavior is true even for liquid systems. The “thermodynamic” formalism has made it possible to get quantitative results for both functions, at least for small enough coupling parameter \( \epsilon \). \( n_\sigma(\bar{v}) \) is linear in \( \bar{v} \) for \( \epsilon = 0 \) and becomes nonlinear for \( \epsilon > 0 \). \( \bar{n}_s(v) \) is already nonlinear in \( v \) in case of \( \epsilon = 0 \). For \( v \) close to \( v_{gs} \) it exhibits a power law. We have shown that this power law behavior is not changed for \( 0 < \epsilon < \epsilon_c \), assuming the ground state to be ferroelastic. For an antiferroelastic ground state one
arrives at the same conclusion. However, whether the power law exists for periodic ground states with period larger than two or even for quasiperiodic ones is not yet clear. In addition, its importance for physically relevant quantities is not obvious.

The fact that functions \( n_s \) and \( \bar{n}_s \) are different, seems to be in variance with the numerical results of Ref. \(^2\). These two functions were found to be the same, within statistical errors. This implies that also \( \bar{n}_s (v) \) vanishes at an energy above \( v_{gs} \). The liquid in Ref. \(^2\) was equilibrated at a temperature, e.g. \( T = 2 \) and 0.5 (in Lennard-Jones units). \( T = 0.5 \) is already close to the mode coupling temperature \( T_c \) where the dynamics is already rather slow. For \( n_s = 0 \) there is a huge variety of stationary points with energies \( v_{gs} \leq v \leq N^{-1}E(\sigma) \) with \( \sigma_n = + \) or \(-\). Their maximum weight occurs when \( N_+ = N_- = N/2 \) (\( N_\sigma \) = number of \( \sigma_n \)'s in \( \sigma \) which are equal to \( \sigma \)). The stationary points with \( n_s = 0 \) which are close to \( v_{gs} \) have an exponentially smaller weight and can only be found at \( T \) much smaller than 0.5 where the configurations look like a crystal with a low concentration of defects. It seems to us unlikely that the simulation done in Ref. \(^2\) which has reached \( T = 0.5 \) from the liquid phase has really been in the range of such defected crystalline configurations. Our result that \( \bar{n}_s (v) \) vanishes at \( v_{gs}, \) only, which implies that \( \bar{n}_s \) as function of temperature vanishes at \( T = 0, \) only, is consistent with recent results \(^22,26\) and second paper of Ref. \(^8\).

Let us come back to a liquid system. How could one apply a similar strategy as used in the present paper? The answer is as follows: Divide the sample with \( mN \) particles into \( m \)-boxes with \( N \) particles where \( 1 \ll m \ll N \). Let us switch off the inter-box interactions. Then the number of stationary points and the saddle index properties can be related to the corresponding quantities of a single box. This starting point corresponds to Aubry’s anti-continuum limit, although a single box represents already a nontrivial problem. Then one can use again the implicit function theorem to prove that the topological features are unchanged under turning on the inter-box interactions, provided their strength is below a critical value. However, increasing this strength such that inter- and intra-box- interactions are the same may exceed the critical strength. As far as we know this type of reasoning has been used first by Stillinger (see \(^22\) and references therein). Recently it has been used again\(^22,26\). Based on independent boxes the authors of Ref. \(^2\) have derived a relationship between \( \alpha, a \) and \( \gamma \) which yield the number of stationary points with saddle index \( n_s = N_s/N \) of a single box:

\[
M_n(n_s = 0) = \exp \alpha N
\]
\[
M_n(n_s = 1/N) = aN \exp \alpha N
\]

and the total number of stationary points of a box:

\[
M_N^{tot} = \exp \gamma N.
\]

This relation is:

\[
\gamma = \alpha + a \ln 2.
\]

Now let us apply this reasoning to our \( \phi^4 \)-model. There it is:

\[
M_N(n_s = 0) = 2^N = \exp(N \ln 2)
\]
\[
M_N(n_s = 1/N) = N \cdot 2^{N-1} = \frac{1}{2}N \exp(N \ln 2)
\]
\[
M_N^{tot} = 3^N = \exp(N \ln 3),
\]
i.e. we find: \( \alpha = \ln 2, \) \( a = \frac{1}{2}, \) and \( \gamma = \ln 3. \) Substituting \( \alpha \) and \( a \) into Eq. \((95)\) we get for its r.h.s.:

\[
\gamma_{r.h.s.} = \frac{3}{2} \ln 2 \simeq 1.039
\]

which is close but not identical to \( \gamma = \ln 3 \simeq 1.098. \) Whether this small discrepancy is a hint that correlations between boxes can be neglected or not, is not obvious.

To conclude, we have demonstrated the usefulness of a one-to-one correspondence between stationary points and symbolic sequences.

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