

# Number of metastable states of a chain with competing and anharmonic $\Phi^4$ -like interactions

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We investigate the number of metastable configurations of a  $\Phi^4$ -like model with competing and anharmonic interactions as a function of an effective coupling constant  $\eta$ . The model has piecewise harmonic nearest-neighbor and harmonic next-nearest-neighbor interactions. The number  $M$  of metastable states in the configuration space increases exponentially with the number  $N$  of particles:  $M \propto \exp(\nu N)$ . It is shown numerically that, outside the previously considered range  $|\eta| < \frac{1}{3}$ ,  $\nu$  is approximately linearly decreasing with  $\eta$  for  $|\eta| < 1$  and that  $\nu=0$  for  $\eta \geq 1$ . These findings can be understood by describing the metastable configurations as an arrangement of kink solitons whose width increases with  $\eta$ .

## I. INTRODUCTION

One of the characteristics of amorphous structures is the existence of a complex energy landscape in the configuration space of a classical  $N$ -particle system with  $N \gg 1$  (cf. Fig. 1). It is believed that the number  $M$  of minima in this space increases exponentially with  $N$ ,

$$M(N) \propto \exp(\nu N), \quad (1)$$

where  $\nu$  is of the order of unity.<sup>1</sup> This feature may influence both static and dynamical properties, such as heat capacity and viscosity. The relaxational behavior of fragile and strong glasses was related to quite different landscapes with many and few metastable configurations, respectively.<sup>2</sup>

To establish a precise relationship between a given topology of a landscape and the physical quantities of the corresponding system is a formidable task and has not yet been accomplished. In this paper we content ourselves with the investigation and characterization of the landscape itself. More precisely the validity of (1) will be investigated for a particular model, which allows one to study the dependence of the *maximum configurational entropy*

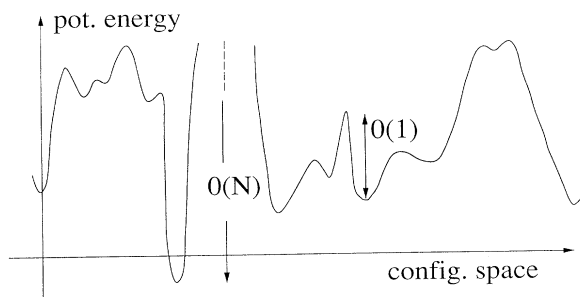


FIG. 1. Schematic representation of the potential-energy landscape.

$$\nu = \lim_{N \rightarrow \infty} \frac{1}{N} \ln M(N) \quad (2)$$

on a coupling parameter. This type of question is already rather difficult and only very few results can be found in the literature. An early study was performed by Hoare and McInnes,<sup>3</sup> who numerically found 36 and 988 metastable configurations for a 13-particle system with Morse and Lennard-Jones potential, respectively. For a soft sphere model with  $r^{-12}$  pair potential, La Violette and Stillinger<sup>4</sup> found  $\nu \cong 0.07$  and—assuming that the prefactor in (1) equals 1—Stillinger and Weber<sup>5</sup> found  $\nu \cong 0.16$  for a modified, finite-range Lennard-Jones system with finite volume and 32 particles.<sup>6</sup> Furthermore, they found a significant increase of  $\nu$  with decreasing density for the latter system.<sup>7</sup> The reliability of these numerical results is not at all clear. There is, for instance, no control whether *all* metastable configurations have been detected.

Under these circumstances simple models, which nevertheless exhibit a complex energy landscape, are useful. The simplest models are chains of particles with *competing* and *anharmonic* interactions such as, e.g., the  $\Phi^4$  model. Another example is a model with piecewise harmonic nearest neighbor and harmonic next-nearest-neighbor interactions as introduced by Reichert and Schilling.<sup>8</sup> Even if it may be pathological for certain physical quantities, it behaves  $\Phi^4$ -like with respect to the number of metastable states. Under certain conditions on the coupling constants *all* metastable configurations are in a one-to-one correspondence to *all* spin configurations of Ising spins  $\sigma_i = \pm 1$ . In this case there are  $2^N$  metastable configurations, and  $\nu = \ln 2$ . Surprisingly, this simple model has some properties in common with glassy materials. For instance, two-level systems and their corresponding density of states were analytically derived, which leads to a power law for the specific heat at low temperatures.<sup>8,9</sup> The spatial decay of the autocorrelation function of the Ising spins is nonexponential.<sup>10</sup> The reader is referred to Ref. 11 for a review of this model and its static and dynamical properties.

For a  $\Phi^4$  model with *infinite*-range interactions (which

can be interpreted as an infinite-dimensional model) a similar relationship between the metastable states and Ising spins has been proven recently.<sup>12</sup> However, permutational invariance of the interactions leads to a high degeneracy of the energies of the metastable configurations, such that the energy landscape is less complex. In contrast to this, the model studied in Ref. 8 has a very complex energy landscape. Häner and Schilling<sup>13</sup> found analytically a maximum stress  $I_{\max}$  such that there are always exponentially many metastable configurations for  $I < I_{\max}$ . The corresponding  $\nu(I)$  shows a staircaselike behavior with an infinite number of plateaux.

In this paper the latter model is used to investigate  $\nu$  as a function of the coupling parameter of the competing interactions together with a properly chosen stress on the chain. Interpreting the  $\Phi^4$ -like model as a coarse grained free energy with *temperature-dependent* coupling constants, the dependence of  $\nu$  leads to a temperature dependence of the number of metastable states in the free-energy landscape. We find that this dependence differs qualitatively from the pressure dependence of  $\nu$ .

There are very few models for which the maximum configurational entropy can be evaluated analytically. Also in the present one, we have to resort to numerical calculations: The quantity  $M(N)$  will be approximated by only evaluating the *periodic* configurations of period  $N$ . It is known that this yields the correct answer in the limit  $N \rightarrow \infty$  but for finite  $N$ , it is difficult to estimate the reliability of the approximation. Therefore, the results are compared with those obtained by a transfer-matrix method, as well as by a formal scattering method due to Kovács and Tél<sup>17</sup> that can be implemented in a closely related dynamical system.<sup>14,8</sup>

This paper is organized as follows. In Sec. II we present the model and discuss some of its crucial properties. Section III deals with numerical methods to determine  $\nu$  approximately. The results deduced from different methods are compared with each other. The underlying physics of the numerical results is elucidated in Sec. IV, where an excellent lower bound to  $\nu$  is obtained by describing metastable configurations as an arrangement of defects in states that are stable for all values of the coupling constant and an upper bound is derived using dynamical system theory. Section V contains a discussion of the results and some conclusions.

## II. THE MODEL

We consider a chain of  $N$  identical classical particles which interact with their nearest- and next-nearest neighbors. The potential energy is given by

$$V(\{v_i\}) = \sum_i [V_1(v_i) + V_2(v_i + v_{i+1})]. \quad (3)$$

$v_i$  may be interpreted either as the bond length between adjacent particles or as a scalar displacement of the  $i$ th particle from a lattice point at  $R_i$ . In the latter case we obtain a type of model that has been intensively studied in the seventies in order to describe phenomena associated with structural phase transitions.<sup>15,16</sup> The former interpretation is useful as a concept for structural glasses

that have been related to spatial chaos.<sup>8,11</sup> In the following we will not distinguish between both interpretations.

For  $V_1$  we choose a piecewise harmonic interaction,

$$V_1(v) = \frac{1}{2}C_1 \{ [v - a_+ - a_- \operatorname{sgn}(v - c)]^2 - [c - a_+ - a_- \operatorname{sgn}(v - c)]^2 \} \quad \text{with } C_1 > 0 \quad (4a)$$

and for  $V_2$  a harmonic one,

$$V_2(v) = \frac{1}{2}C_2[v - b]^2 \quad \text{with } C_2 \neq 0. \quad (4b)$$

$C_1$  and  $C_2$  are elastic constants and the other model parameters become obvious from Fig. 2.

Let us repeat some of the most important properties of this model (details can be found in Refs. 8 and 11). The metastable configurations at  $T = 0$  K (not to be confused with metastable phases at finite temperatures  $T > 0$  K) are of particular interest. A configuration  $\{v_i\}$  of the chain with internal stress  $I$  is metastable if it is a stationary configuration:

$$\frac{\partial V}{\partial v_n}(\{v_i\}) = I \quad \text{for all } n, \quad (5)$$

and if the phonon frequencies are non-negative, i.e., the Hessian matrix is positive semidefinite. Due to the piecewise harmonic potential  $V_1$ , it is easy to prove that the second condition holds for *all* stationary configurations, provided that  $C_1 > 0$  and  $C_2 > -C_1/4$ . For smaller values of  $C_2$ , there are only unphysical configurations with  $v_i \equiv \pm \infty$ .

Analogous to the discussion in Ref. 8, the first condition gives rise to the nonlinear difference equation

$$2\gamma(v_n - c) + (v_{n-1} - c) + (v_{n+1} - c) = \Phi(v_n - c), \quad (6a)$$

with

$$\Phi(x) = -(2\gamma + 2)c + \frac{I}{C_2} + 2b + 2(\gamma - 1)[a_+ + a_- \operatorname{sgn}(x)] \quad (6b)$$

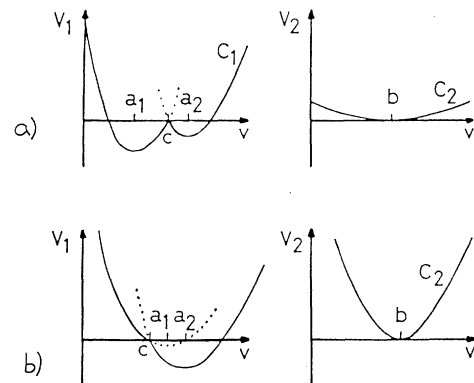


FIG. 2. Nearest- and next-nearest-neighbor potential; (a) double-well-like potential, (b) single-well potential.  $a_+$  and  $a_-$  are related to  $a_{1,2}$  by  $a_{\pm} = (a_2 \pm a_1)/2$ .

and

$$\gamma = 1 + \frac{C_1}{2C_2}. \quad (6c)$$

Note that  $\Phi(v_n - c)$  is a nonlinear function of  $(v_n - c)$  and depends parametrically on the model parameters and on the internal stress  $I$ .

Using a Green's-function method for the infinite chain, (6) can be rewritten as

$$v_n(\{\sigma_i\}) - c = A + B \sum_{i=-\infty}^{\infty} \eta^{|i|} \sigma_{n+i}, \quad (7a)$$

with

$$\eta = -\gamma[1 - (1 - \gamma^{-2})^{1/2}] \quad (7b)$$

and the self-consistency condition (SCC)

$$\sigma_n = \text{sgn}[v_n(\{\sigma_i\}) - c]. \quad (8)$$

In the following, the internal stress  $I$  is adjusted to such a value that

$$A = 0, \quad (9a)$$

$$B = a_- (1 - \eta)^{-1} (1 + \eta), \quad (9b)$$

$$\Phi(v_n - c) = -\eta^{-1} (1 + \eta)^2 a_- \text{sgn}(v_n - c). \quad (9c)$$

It follows immediately from (7) and (9a) that the SCC is invariant under the transformation  $\sigma_i \rightarrow -\sigma_i$ . This symmetry is not crucial, but it is convenient from a technical point of view. Although the symmetry does not hold for arbitrary stress we believe that the  $\eta$  dependence of  $\nu$  does not change qualitatively in that case.

Equation (7) states that the metastable configurations are uniquely characterized by the location of the particles relative to the cusp of  $V_1$ . Thus, each metastable state can uniquely be characterized by a double-infinite sequence of pseudospins  $\sigma_i = \pm 1$ . Its energy, written in terms of the spin variables, has the form of the energy of a 1d Ising model where  $\ln \eta$  takes the meaning of the length scale of the spin-spin interaction.<sup>8</sup> In Sec. IV, the language of spin chains will be used to derive an analytical lower bound for the configurational entropy.

For a given sequence  $\{\sigma_i\}$  the solution (7) has to fulfill the SCC (8). In Ref. 8 it was shown that this is true for *all* sequences, provided that  $|\eta| < \frac{1}{3}$ . In that case the number of metastable configurations

$$M(N, \eta) = \text{card}\{\{\sigma_i\} | \{\sigma_i\} \text{ fulfills (8) for all } n\} \quad (10)$$

is given by

$$M(N, \eta) = 2^N. \quad (11)$$

For  $|\eta| > \frac{1}{3}$  we expect  $M(N, \eta)$  to decrease with increasing  $|\eta|$ . The critical value  $\eta_c = \frac{1}{3}$  corresponds to the critical  $\mu_c = \frac{1}{3}$  in the model of Ovchinnichov and Onischyk,<sup>12</sup> but the coincidence of the numerical values is fortuitous.

Since the condition  $C_1 > 4|C_2|$  for metastability implies  $|\eta| < 1$  we have to investigate  $M(N, \eta)$  for  $\frac{1}{3} \leq |\eta| \leq 1$  only. Without loss of generality we choose  $\eta > 0$ . The case  $\eta < 0$  can be reduced to positive  $\eta$  by the transforma-

tion  $\sigma_{2n} \rightarrow \sigma_{2n}$  and  $\sigma_{2n+1} \rightarrow -\sigma_{2n+1}$ , due to the choice of the internal stress.

### III. NUMERICAL METHODS AND RESULTS

The main problem in calculating  $M(N, \eta)$  from (8) is the *nonlocality* of the self-consistency condition, i.e., the impossibility to evaluate the infinite sum in (7) exactly. One has to approximate the problem in such a way that the sum can be evaluated. This has been done by imposing periodic boundary conditions on the chain. Thus, the infinite sum of the SCC reduces to  $N$  terms only and for a fixed period  $N$ , at most  $2^N$  sequences need to be investigated.

Period- $N$  configurations are defined by  $v_{n+N} = v_n$  or equivalently by  $\sigma_{n+N} = \sigma_n$  for all  $n$ . Subsequently the infinite sum involved in the SCC reduces to a rational function of degree  $N$  in  $\eta$ ,

$$P_N(\sigma_0 \dots \sigma_{N-1}; \eta) = \frac{1}{2} \frac{1 - \eta}{1 - \eta^N} \sum_{k=0}^{N-1} (\eta^k + \eta^{N-k}) \sigma_k, \quad (12)$$

and the SCC becomes

$$\sigma_n = \text{sgn} P_N(\sigma_n \sigma_{n+1} \dots \sigma_{n+N-1}; \eta). \quad (13)$$

A periodic sequence described by the "unit cell"  $(\sigma_0 \dots \sigma_{N-1})$  is allowed if and only if (13) is satisfied for  $n = 0, \dots, N-1$ . Only in this case, it represents a metastable configuration. Since all sequences are allowed for  $\eta = 0$ , a periodic sequence is not allowed if

$$\text{sgn} P_N(\sigma_{i_1} \dots \sigma_{i_N}; \eta) \neq \text{sgn} P_N(\sigma_{i_1} \dots \sigma_{i_N}; 0) \quad (14)$$

for any cyclic permutation of  $(\sigma_0 \dots \sigma_{N-1})$ . The configuration is forbidden for  $\eta > \eta_c(\sigma_0 \dots \sigma_{N-1})$ , where  $\eta_c$  is the smallest zero of any of the polynomials  $P_N(\sigma_{i_1} \dots \sigma_{i_N}; \eta)$  (cf. Fig. 3). The determination of zeros of  $P_N$  is done numerically. For fixed  $N$  one can decide after one computer run for *any* periodic configuration up to which value  $\eta_c$  it is allowed. The symmetry between  $\sigma_i$  and  $-\sigma_i$  reduces the numerical effort. Table I shows the number of unrelated sequences  $(\sigma_1 \dots \sigma_N)$  which have to be checked and the corresponding number of roots for several  $N$ . Given  $\eta$ , the number of allowed

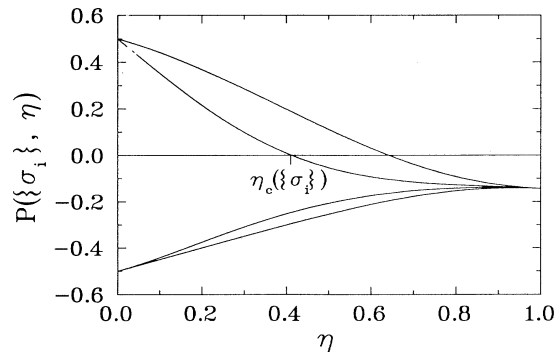


FIG. 3. The polynomials involved in the SCC for the periodic configuration  $\{\sigma_i\} = (1, 1, -1, -1, 1, -1, -1)$  and its cyclic permutations.

TABLE I. Number of polynomials to check when evaluating the consistency condition for periodic configurations.

Period length	Number of different configurations	Roots to find
10	39	390
15	607	9105
20	13 602	272 040
21	25 472	534 912

period- $N$  configurations approximates  $M(N, \eta)$ . The result for  $\nu(N, \eta)$  is displayed in Fig. 4 for several values of  $N$ .

Near  $\eta = \frac{1}{3}$  the curves for different  $N$  coincide, whereas large discrepancies exist in the limit  $\eta \rightarrow 1^-$ . This is quite natural, as the number of allowed configurations is rapidly decreasing with  $\eta$ , so that the statistics becomes bad in this limit. Moreover calculations with even  $N$  overestimate  $M(\eta)$ , as untypically many extremely stable kink configurations (cf. Sec. IV) contribute in this case. This effect becomes most severe in the limit  $\eta \rightarrow 1^-$ .

Since it is difficult to estimate the error of the results for large  $\eta$ , the latter have been compared to results obtained by two other methods: a *transfer-matrix method*<sup>13</sup> and a “*scattering method*”.<sup>17,18</sup>

The transfer-matrix method operates on the whole set of all sequences. Truncating the sum in (7) at  $|i|=k$  reduces the SCC to a local problem.<sup>13</sup> This approximation allows to determine finite forbidden subsequences of length  $2k+1$ . An infinite sequence is said to be forbidden at level  $k$  if it contains at least one forbidden block of length  $l \leq 2k+1$ . It has been shown<sup>13</sup> that  $\nu$  is approximately given as logarithm of the largest eigenvalue of a  $2^{2k+1}$ -dimensional transfer matrix, which operates on the set of subsequences of length  $2k+1$ .

The scattering method is in some sense complementary to the preceding one. Only finite symbol sequences are considered, but the SCC is evaluated exactly. Being inspired by numerical scattering experiments,<sup>17</sup> it consists in determining finite allowed symbol sequences of length  $N$ , by fixing  $v_0$  and  $v_{-1}$  to some appropriate value and

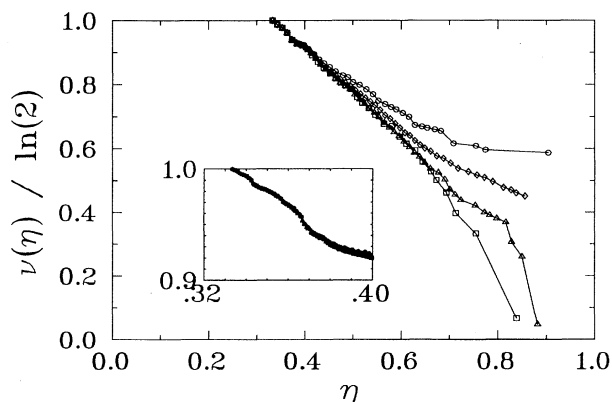


FIG. 4. Numerical results for the maximum configuration entropy  $\nu$  when approximating the configurations by periodic ones; ( $\circ$ )  $N=14$ ; ( $\square$ )  $N=15$ ; ( $\diamond$ )  $N=20$ ; ( $\triangle$ )  $N=21$ .

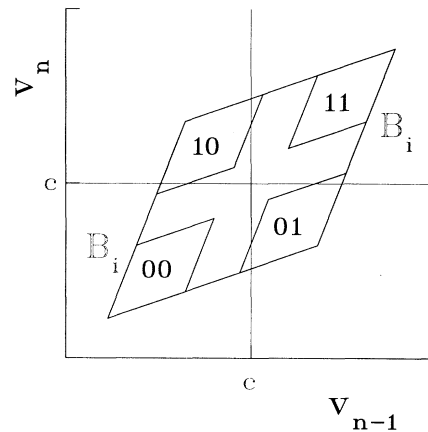


FIG. 5. Invariant set of the two-dimensional (2D) map that is constructed in such a way that any orbit in its invariant set corresponds one-to-one with a metastable configuration of the chain. The instable boundaries are labeled by  $B_i$ . For details of the construction the reader is referred to Ref. 11.

checking if the SCC is satisfied exactly for all  $i \leq N$ . This corresponds to investigating finite configurations with one end fixed. The initial conditions must be located on the instable boundaries of the invariant set of the related two-dimensional map (cf. Fig. 5).<sup>17,18</sup> Since  $v_i$  is calculated by (6) and not by a truncation of (7), no approximation is made in the evaluation of the SCC.

In the limit of large  $N$  for the first and the third approach, and large  $k$  for the second approach, all methods converge to the same value for  $\nu$ . Their rate of convergence is nevertheless different, and there are advantages

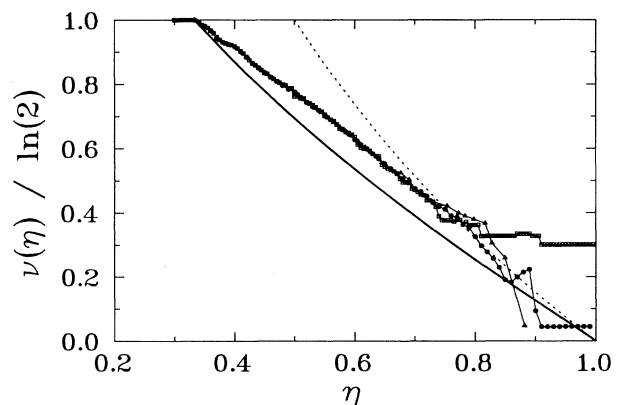


FIG. 6. Survey over the results for the maximum configuration entropy  $\nu$  obtained by different numerical and analytical methods; ( $\triangle$ ) numerical calculation by periodic configurations with  $N=21$ ; ( $\square$ ) numerical calculation by the transfer-matrix method with  $k=7$ ; ( $\bullet$ ) numerical calculation by the scattering technique with  $N=16$  for  $\frac{1}{3} < \eta < 0.5$ ,  $N=20$  for  $0.5 \leq \eta < 0.65$ , and  $N=30$  for  $\eta \geq 0.65$ ; (solid line) analytical lower bound for  $\nu$  by counting the number of allowed kink states; (dotted line) analytical upper bound by a connection between  $\nu$  and the fractal dimension of the invariant set of the 2D map.

and shortcomings due to conceptual differences between them.

In Fig. 6 the numerical results of the three methods are compared. For  $\eta \lesssim 0.7$ , the predictions of the different calculations are in excellent agreement. In this range, the errors of all the methods are small.

The scattering method allows more easily than the other ones to approximate a metastable state by longer symbol sequences (length of 30 instead of 15 for transfer matrices and 21 for periodic configurations). Moreover, there is the possibility to include finite-size scaling into the calculations. These data can be expected to be the most reliable ones for relatively high values of  $\eta$ . According to these data,  $\nu(\eta)$  is, in a first approximation for the range  $0.4 < \eta < 1$ , a linearly decaying function of  $\eta$  which vanishes for  $\eta=1$ . The linear approximation seems to be quite good for  $\eta > \frac{1}{2}$ , but due to the resolution of our calculations it is difficult to get detailed information on its quality. In contrast there are outspoken deviations from linear decay for  $\frac{1}{3} < \eta < \frac{1}{2}$ . Using the good resolution of periodic configurations with  $N=21$  to plot  $\log_{10}[\ln 2 - \nu(\eta)]$  against  $\log_{10}(\eta - \frac{1}{3})$ , one discovers that these deviations are due to a scaling law for the number of orbits to be forbidden at a certain value of  $\eta$ . This law also fixes the asymptotic behavior of  $\nu(\eta)$  for  $\eta \rightarrow \frac{1}{3}^+$ .<sup>19</sup>

#### IV. DEFECT METHOD

In this section we present analytical methods for the calculation of a lower and an upper bound of  $\nu(\eta)$ . The calculation of the lower bound elucidates the physical mechanism that leads to the decrease of  $\nu$  with increasing effective coupling constant  $\eta$ . An upper bound is derived using a formal argument from the theory of dynamical systems. Both bounds converge in the limit  $\eta \rightarrow 1^-$ . Thus, it is possible to verify the numerical finding that  $\nu$  vanishes linearly in this limit.

Let us begin the derivation of the lower bound with the remark that both "ferromagnetic" spin configurations,  $\{\sigma_i = +1\}$  and  $\{\sigma_i = -1\}$ , fulfill the SCC up to  $\eta=1$ . For our choice of the internal stress and for  $\eta > 0$ , these two configurations represent the twofold degenerate ground states. An elementary defect is an Ising domain wall defined by

$$\sigma_n = \begin{cases} -1, & \text{for } n < n_0 \\ +1, & \text{for } n \geq n_0 \end{cases}, \quad (15)$$

where  $n_0 - \frac{1}{2}$  is its position. For this defect configuration the SCC holds up to  $\eta=1$ . Substituting (15) into (7) we obtain

$$v_n = c + \sigma_n B \left\{ \frac{1+\eta}{1-\eta} - 2 \frac{\eta^{1/2}}{1-\eta} \right. \\ \left. \times \exp \left[ - \left| n - n_0 - \frac{1}{2} \right| \ln \left[ \frac{1}{\eta} \right] \right] \right\}. \quad (16)$$

Hence the defect width is

$$w(\eta) = \left[ \ln \left[ \frac{1}{\eta} \right] \right]^{-1}. \quad (17)$$

Now, let us consider a configuration with a pair of defects at  $n = -\frac{1}{2}$  and  $n = l + \frac{1}{2}$ :

$$\sigma_n = \begin{cases} -1, & \text{for } 0 < n < l + 1 \\ +1, & \text{otherwise} \end{cases}. \quad (18)$$

This configuration describes a finite domain of  $l$  minus signs in an infinite domain of plus signs. The SCC is fulfilled only for  $\eta$  with

$$1 - \eta - 2\eta^l \geq 0, \quad (19)$$

as can be verified by inserting (18) into (7) and using constants as given in Eqs. (9a) and (9b) to explicitly check (8). Doing this one observes that spins adjacent to the defects first violate the SCC and that both defects in (18) lead to the same critical value  $\eta$ .

Note that  $l=1$  yields the critical value  $\eta_c = \frac{1}{3}$ . For  $\eta > \frac{1}{3}$  the inequality can only be satisfied for  $l > l_0(\eta)$ , where

$$l_0(\eta) = \ln \left[ \frac{2}{1-\eta} \right] w(\eta). \quad (20)$$

Since  $\ln[2/(1-\eta)]$  grows rapidly with  $\eta$ , the distance between the defects has to increase faster than the defect width  $w(\eta)$ , in order that the SCC holds. Since the number  $M$  of metastable configurations is related to the number of defects, it is obvious that  $M$  decreases with  $\eta$  due to the decrease of the defect concentration. This relationship will be worked out now.

Equation (20) defines a critical value  $\eta_l$  for given  $l$ . At  $\eta_l$  all configurations composed of plus and minus domains with size  $l' \geq l$  are allowed. Thus,  $M(N, \eta_l)$  is the number of possibilities to decompose  $N$  into blocks of size  $l' \geq l$ . This is a well-known problem from combinatorics. One obtains<sup>20</sup>

$$M(N, \eta) \propto \alpha^N, \quad (21)$$

i.e.,

$$\nu(\eta) = \ln(\alpha) \quad (22)$$

for  $\eta = \eta_l$ , where  $\alpha$  is the largest (with respect to its modulus) zero of the polynomial

$$x^l - x^{l-1} - 1 = 0. \quad (23)$$

Eliminating  $l$  from (19) and (23), an implicit equation for  $\ln \alpha(\eta)$  is found:

$$\ln \alpha = \frac{\ln \eta}{\ln \eta - \ln[(1-\eta)/2]} \ln(\alpha - 1). \quad (24)$$

Its numerical solution leads to the  $\nu(\eta)$  curve shown in Fig. 6 by the solid line.

Besides  $\{\sigma_n = +1\}$  and  $\{\sigma_n = -1\}$  there are many more configurations that are metastable up to  $\eta=1$  [e.g., any  $2N$ -periodic alternating configuration  $\sigma_i = +1$ , for  $2nN \leq i < (2n+1)N$  and  $\sigma_i = -1$  otherwise]. These configurations and those that can be related to them by

inserting defects are neglected. Therefore, the above result for  $\nu(\eta)$  is only a lower bound.

An upper bound is obtained by the following reasoning: The metastable states of the chain correspond to the orbits in the invariant set of a two-dimensional map.<sup>11</sup> In this picture any allowed *finite* sequence  $\{\sigma_i\}_{i=1}^N$  uniquely corresponds to a square with side length  $\eta^{N/2}$ . The position of the square is uniquely determined by the symbols  $\sigma_i$  (cf. Fig. 5). This means that the invariant set is an “incomplete Cantor set” with scaling  $\eta$  and a fractal dimension  $D$ .  $M(N)$  corresponds to the number of boxes with side length  $\eta^{N/2}$  in the Cantor set,<sup>21</sup> i.e.,

$$M(N) = (\eta^{N/2})^{-D}. \quad (25)$$

Here,  $M(N)$  denotes the number of allowed sequences of length  $N$ , as it is given in (1). Using (2) and observing that the dimension of the invariant set of a two-dimensional map can never exceed 2, one obtains

$$\nu = \lim_{N \rightarrow \infty} \frac{1}{N} \ln(\eta^{-DN/2}) = -\frac{D}{2} \ln \eta \leq -\ln \eta. \quad (26)$$

This upper bound is given by the dotted line in Fig. 6. Note that both bounds are tangent in the limit  $\eta \rightarrow 1^-$ , proving that  $\nu$  vanishes linearly with slope  $-1$ :

$$\nu(\eta) = 1 - \eta + O(1 - \eta)^2 \quad \text{for } \eta \rightarrow 1^-. \quad (27)$$

## V. DISCUSSION AND CONCLUSIONS

In this paper we have investigated the number  $M(N, \eta)$  of metastable configurations of a chain of  $N$  particles with competing and anharmonic interactions as a function of an effective coupling constant  $\eta$ . For  $\eta < \frac{1}{3}$  it had already been shown that  $\nu(\eta) = \ln 2$ . For  $\frac{1}{3} \leq \eta \leq 1$  three different numerical methods yield an approximately linear decrease of  $\nu$  with increasing  $\eta$ .

In addition we have described the metastable configurations as an arrangement of defects. For  $\frac{1}{3} < \eta \leq 1$  the spacing between adjacent defects has to exceed a critical length  $l_0(\eta)$ . Counting all configurations of defects with neighboring distance bigger than  $l_0$ , we find a lower bound for  $\nu(\eta)$ , which is exact for  $\eta = \frac{1}{3}$  and takes the value 0 for  $\eta = 1$ . Using a mapping of this problem to a dynamical system, an upper bound for  $\nu(\eta)$  has been derived. Both bounds are tangent at  $\eta = 1$ , proving that  $\nu(\eta)$  vanishes linearly with slope  $-1$ . For  $\eta > 1$  it has previously been shown that  $\nu = 0$ .<sup>8</sup>

The  $\Phi^4$  model with infinite-range interaction studied by Ovchinnikov and Onisych<sup>12</sup> also exhibits an energy

landscape with exponentially many metastable configurations, which are classified by Ising-spin configurations. For this model one can show that spin configurations  $\{\sigma_i\}$  for which  $\sum_i \sigma_i = 0$  represent metastable configurations for *all* values of the coupling constant. In the thermodynamic limit  $N \rightarrow \infty$  they constitute the full measure. Therefore,

$$\nu \equiv \ln 2 \quad (28)$$

for *all* coupling parameters.

The reason for this trivial  $\eta$  dependence in contrast to  $\nu(\eta)$  for our model may be explained as follows. In case of infinite-range interactions the force acting on a particle  $n$  depends only on the “magnetization”  $\sum_i \sigma_i$ , i.e., it is independent of  $n$ , whereas for the chain of particles the force is proportional to  $\sum_i \eta^{|n-i|} \sigma_i$ . Any permutation of the  $\sigma_i$  changes the force in case of the chain. Therefore, the high degeneracy of the infinite-range model is removed. In particular, the energies of the  $\binom{N}{N/2}$  configurations with  $\sum_i \sigma_i = 0$  (for  $N$  even) are spread over the full energy scale. Increasing  $\eta$ , one configuration after the other will become unstable leading to a decrease in  $\nu$ . It is not obvious to us why the decay is approximately linear. It would be interesting to compare our results with a true  $\Phi^4$  model with finite-range interactions.

Compared with the pressure-dependence for  $\eta < \frac{1}{3}$ ,<sup>13</sup> the  $\eta$  dependence of  $\nu$  presents significant differences. In the former case an infinite number of plateaus exists where  $\nu(p)$  is constant. Our results for  $\nu(\eta)$  do not give any evidence for the existence of plateaus for  $\frac{1}{3} \leq \eta \leq 1$ . We believe that the number of metastable configurations changes continuously and *strictly* monotonically with  $\eta$  and that consequently the quality of the energy landscape changes “smoothly.”

To summarize, the energy landscape of the one-dimensional model exhibits exponentially many local minima (metastable configurations) for  $\eta < 1$ . The corresponding maximum configurational entropy  $\nu$  decreases roughly linearly for  $\frac{1}{3} < \eta < 1$ . The description of metastable configurations by defects is appealing and may in principle be extended to more general systems.

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