Saddle index properties, singular topology, and its relation to thermodynamic singularities for a ϕ^4 mean-field model

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We investigate the potential energy surface of a ϕ^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 μ is smaller than a critical value. The saddle index n_s is equal to α_0 and its distribution function has a maximum at $n_s^{\max} = 1/3$. 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, $e_c(\mu) \neq v_c(\mu)$, where $v_c(\mu)$ 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 $\overline{n_s}$ 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 $\overline{e}(n_s)$ is given by $n_s(\overline{e}) = 1 + 4\overline{e}$ (for $H = 0$) that vanishes at $\overline{e} = -1/4 > v_0$, the ground state energy.

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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 ϕ^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, v_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 [6,7] 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 χ [3,4,9] which is a topological invariant. For the two-dimensional nearest neighbor ϕ^4 model [10], the mean-field *XY* [11] and mean-field *k*-trigonometric model [12,13] it was proven that $\chi(e)$ also becomes singular at $e_c = v_c$. 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 $\leqslant e$ and saddle index $n_s = N_s/N$ [9],

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

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 $N \gg 1$,

$$M(e, N_s) \sim \exp[Ns(e, n_s)], \tag{2}$$

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

$$p(e, n_s) = \frac{\partial}{\partial e} M(e, N_s) \sim \exp[Ns(e, n_s)]. \tag{3}$$

The relationship between Eqs. (1) and (3) 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

$$\overline{n_s}(e) = \int_0^1 dn_s \, n_s p(e, n_s) \tag{4}$$

and the average energy for a fixed value of n_s,

$$\overline{e}(n_s) = \int_{-\infty}^{\infty} de\, e\, p(e,n_s). \tag{5}$$

In the limit $N\to\infty$ the averages $\overline{n_s}(e)$ and $\overline{e}(n_s)$ are simply the values that maximize the configurational entropy, i.e., they are solutions of the equations

$$\frac{\partial s}{\partial n_s}(e,\overline{n_s}) = 0, \quad \frac{\partial s}{\partial e}(\overline{e},n_s) = 0. \tag{6}$$

The saddle index properties of a PES have also played an important role in another respect. Studying *glassy dynamics* and ideal *dynamical glass transition* [14] for liquids it has been found numerically [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 [14]. However, this conclusion should be taken with some care. First of all most saddle points were quasisaddles (see the discussion in Refs. [17–19]) and second, plotting $\log \overline{n_s}(T)$ (or a related quantity) versus $1/T$ does not exhibit a quasisingular behavior at T_c [20,21]. That $\overline{n_s}(T)$ vanishes at $T=0$, only, has been proven for the *k*-trigonometric model [13]. This indicates that $\overline{n_s}(T)$ for systems with *self-generated* disorder behaves differently than for systems where the disorder is *quenched.* For the latter it has been proven that $\overline{n_s}(T)$ vanishes at the dynamical transition point, at least for mean-field-like models [22].

A numerical determination of the *true* saddles of a binary liquid with particle number $N\leqslant 13$ gives evidence that $\overline{n_s}(e)$ vanishes at an energy e^*, which still depends on N [17]. This evidence holds for both cases where the average $\overline{n_s}$ is plotted versus e and n_s is plotted versus $\overline{e}$ [17]. Whether this vanishing at e^* is spurious or not is not known. It is obvious why vanishing of $\overline{n_s}$ 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 flowlike. Hence, vanishing of $\overline{n_s}(e)$ may indicate a qualitative change in the dynamics [15,16].

There is another result presented in Ref. [17] which concerns the distribution function of the saddle index $p(n_s)$,

$$p(n_s) = \int_{-\infty}^{\infty} de\, p(e,n_s). \tag{7}$$

It is found that $p(n_s)$ is a Gaussian with a maximum at $n_s^{\max}\approx 1/3$. 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* ϕ^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 ϕ^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 ϕ^4 MODEL

Let x_n be a scalar displacement of a particle from a lattice site n. We consider the following potential energy:

$$V(\mathbf{x},H) = \sum_{n=1}^{N} V_0(x_n,H) - \frac{\mu}{2N}\left(\sum_{n=1}^{N} x_n\right)^2 \tag{8}$$

depending on the N-particle configuration $\mathbf{x}=(x_1,\ldots,x_N)$. $V_0(x,H)$ is an asymmetric on-site potential,

$$V_0(x,H) = -xH - \tfrac{1}{2}x^2 + \tfrac{1}{4}x^4, \tag{9}$$

that becomes symmetric for $H=0$. The final term in Eq. (8) represents the harmonic interaction between *all* particles with a coupling parameter $\mu\geqslant 0$. 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. (9). This type of model was used to describe structural phase transitions [23]. In contrast to the mean-field models studied in Refs. [8,11–13] there is a nontrivial coupling constant μ, which cannot be put to one by an appropriate scaling of the temperature.

Some thermodynamic properties of the model described by Eqs. (8) and (9) as well as some features of its PES were already investigated [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 $\langle x\rangle=\langle x_n\rangle(T,H)$,

$$\langle x\rangle = \frac{1}{\mathcal{Z}}\int_{-\infty}^{\infty} dx\, x \exp\left[-\frac{V_0(x,H)-\mu\langle x\rangle x}{T}\right], \tag{10}$$

where $\mathcal{Z}$ 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

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

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

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

which yields for the average potential energy per particle $\overline{v}(T)=\lim_{N\to\infty} N^{-1}\langle V(\mathbf{x})\rangle(T,H=0)$ at T_c

$$v_c = v(T_c) = -\tfrac{1}{4}(1-2\mu) + \mathcal{O}(\mu^2) \tag{13}$$

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

$$H_{\rm int} = \frac{\mu}{N}\sum_{n=1}^{N} x_n \tag{14}$$

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

$$x^3 - x - H_{\rm eff} = 0 \tag{15}$$

with the effective field [25]

$$H_{\rm eff} = H + H_{\rm int}. \tag{16}$$

For $|H_{\rm eff}| < H_c = 2/(3\sqrt{3})$ there are three real roots of Eq. (15) which will be denoted by $x_\sigma(H_{\rm eff})$, $\sigma = +,0,-$. It is $x_+ > x_0 > x_-$. A stationary point of V is characterized by N_σ, the number of x_n in $\mathbf{x}$ which are equal to $x_\sigma(H_{\rm eff})$. 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

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

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

$$\sum_\sigma N_\sigma = N, \tag{18}$$

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

$$\alpha_\sigma = \frac{N_\sigma}{N}, \quad \sum_\sigma \alpha_\sigma = 1 \tag{19}$$

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

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

[We omit the arguments H and μ for brevity and we take into account that α_- can be expressed by α_+,α_0, due to Eq. (19). Also we will mostly drop the arguments (α_+,α_0) of $H_{\rm eff}$.] Finally the stationary points of class (N_+,N_0,N_-) are given by

$$\mathbf{x}(H_{\rm eff}) = (\underbrace{x_+(H_{\rm eff}),\cdots}_{N_+ \text{ times}};\ \underbrace{x_0(H_{\rm eff}),\cdots}_{N_0 \text{ times}};\ \underbrace{x_-(H_{\rm eff}),\cdots}_{N_- \text{ times}}).$$

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

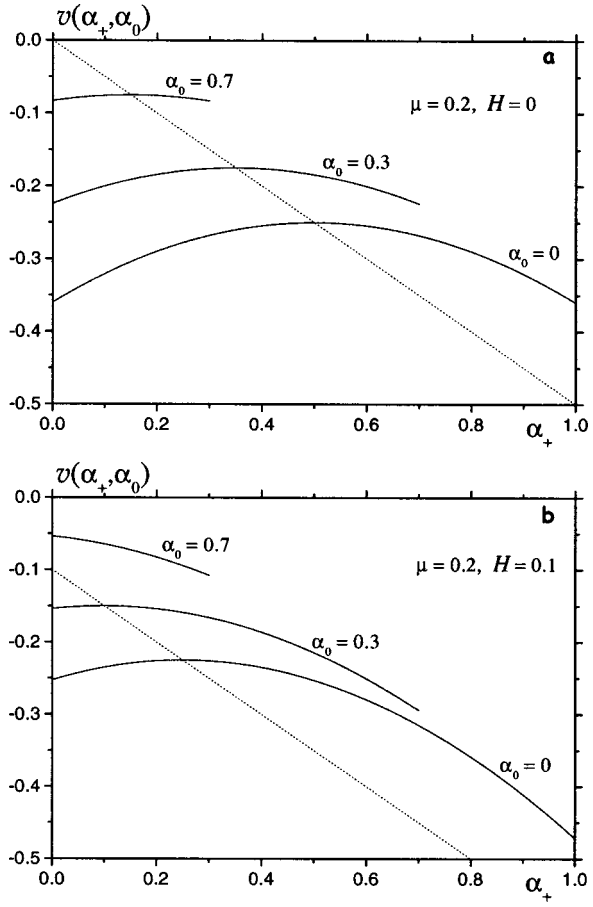

FIG. 1. (a) α_+ dependence of $v(\alpha_+,\alpha_0)$ for $\mu=0.2$ and $H=0$; (b) same for $H=0.1$. Dotted lines locate the maxima. Note the concavity of $v(\alpha_+,\alpha_0)$ in α_+ for $H \geqslant 0$ and its symmetry with respect to the maximum position $\alpha_+^{\rm max} = (1-\alpha_0)/2$ for $H=0$.

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

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

Equation (21) holds for $|H_{\rm eff}| \leqslant H_c$. One can easily prove that the latter is guaranteed for arbitrary $\{\alpha_\sigma\}$ with $\Sigma_\sigma \alpha_\sigma = 1$ if

$$-H_c(1-3\mu) \leqslant H \leqslant (1-3\mu)H_c. \tag{22}$$

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 $\{\alpha_\sigma\}$ [26]. Therefore we will restrict ourselves to $\mu \leqslant 1/3$, 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

$$n_s \equiv \alpha_0. \tag{23}$$

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. (23). Validity of Eq. (23) can also

be seen as follows. If $\mu=0$ and $H\geqslant 0$, 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 $0\leqslant\mu<1/3$. Consequently Eq. (23) 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 ϕ^4 model are characterized by $\{\alpha_\sigma\}$, 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):

$$p(n_s)=3^{-N}\sum_{N_+=0}^{N-N_s}P(N_+,N_s)=\frac{3^{-N}2^{N-N_s}N!}{N_s!\,(N-N_s)!}. \tag{24}$$

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

$$s(n_s)=-\left[n_s\ln n_s+(1-n_s)\ln\frac{1-n_s}{2}\right]. \tag{25}$$

The maximum of $p(n_s)$ is at $n_s^{\max}=1/3$ which is obvious since $P(N_+,N_0)$ has a maximum at $N_+=N_0=N_-\equiv N/3$. It is interesting that this result based on the double-well character of the local potential, coincides with the numerical finding for binary Lennard-Jones clusters [17]. We stress that the validity of $n_s^{\max}=1/3$ 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. (17). 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, $n_s^{\max}=1/3$ 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

$$p(e,n_s)=\sum_{N_+=0}^{N-N_0}P(N_+,N_0)\,\delta(v(\alpha_+,\alpha_0)-e), \tag{26}$$

where $P(N_+,N_0)$ is given by Eq. (17) 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

$$p(e)=\sum_{N_0=0}^{N}p(e,n_s), \tag{27}$$

Neglecting the irrelevant prefactor one can immediately write $(\alpha_0=n_s)$

$$p(e,n_s)\sim P(N_+(e,\alpha_0),N_0), \tag{28}$$

where $N_+(e,\alpha_0)=\alpha_+(e,\alpha_0)N$ follows from the solution of the equation

$$v(\alpha_+,\alpha_0)=e. \tag{29}$$

This equation has two solutions $\alpha_+^{\pm}(\alpha_0,e)$ 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. (3) with the configurational entropy given by

$$s(e,\alpha_0)=-\alpha_0\ln\alpha_0-\alpha_+^{(+)}\ln\alpha_+^{(+)}-\alpha_-^{(+)}\ln\alpha_-^{(+)}, \tag{30}$$

where $\alpha_-^{(+)}=1-\alpha_0-\alpha_+^{(+)}$ and we have taken the (+) branch of Eq. (B1) 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. (3) only in the energy window

$$v_{\min}(\alpha_0)\leqslant e\leqslant v_{\max}(\alpha_0), \tag{31}$$

where $v_{\min}(\alpha_0)=v(1-\alpha_0,\alpha_0)$ (see Fig. 1) and $v_{\max}(\alpha_0)$ 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

$$\alpha_0^{(\min)}(e)\leqslant\alpha_0\leqslant\alpha_0^{(\max)}(e), \tag{32}$$

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

$$\alpha_0^{(\min)}(e)=1+4e-2H^2/\mu, \tag{33}$$

whereas $\alpha_0^{(\max)}(e)$ can be found with the help of Eq. (21) or, approximately, with the help of Eq. (A5). 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(a)]. The maximum of $s(e,n_s)$ with respect to n_s is denoted by $\overline{n_s}(e)$. 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 $\overline{n_s}(e)$ is identical to the averaged saddle index $\overline{n_s}(e)$ 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 $e\geqslant e_c(\mu)$. 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. Figure 3(a) presents $\overline{n_s}(e)$ and reveals the singularity at $e_c(\mu)$. Note that $\overline{n_s}(e)$ contains a branch that is independent of the interaction [see Eqs. (B6) and (B7)]. For e very close to the

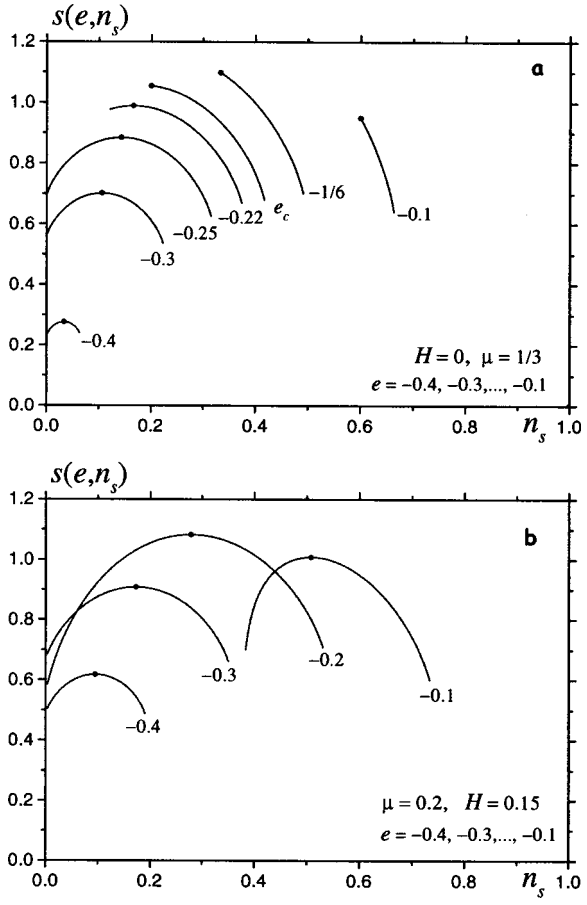

FIG. 2. (a) Configurational entropy $s(e,n_s)$ versus n_s for different energies and zero field; (b) same for nonzero field.

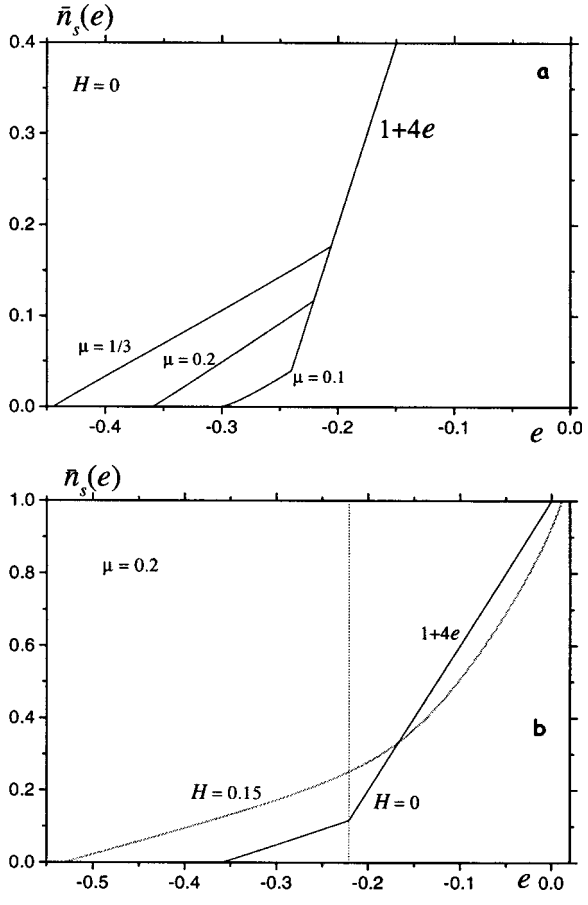

FIG. 3. (a) Averaged saddle index $\overline{n_s}(e)$ versus e for $\mu=0.1,0.2,1/3$ and $H=0$; (b) same for $\mu=0.2$ and $H=0$ and $H=0.15$.

ground state energy $v_0(\mu)$ [cf. (A6)] one obtains the power-law behavior

$$\overline{n_s}(e) \sim [e - v_0(\mu)]^{\delta(\mu)} \tag{34}$$

with $\delta(\mu)>1$, if μ is small enough. Note that $\overline{n_s}(e)\to 0$ for $e\to v_0(\mu)$. The averaged saddle index $\overline{n_s}(e)$ takes the critical value $n_s^{(c)}(\mu)=\overline{n_s}(e_c(\mu))$ shown in Fig. 4. This figure also includes the asymptotic result of Eq. (B5) for $\mu\to 0$.

Instead of fixing e, one can also determine the maximum position $\overline{e}(n_s)$ of $s(e,n_s)$ for given n_s. $\overline{e}(n_s)$ is the averaged saddle energy [cf. Eq. (5)] as function of n_s. It is easy to get $\overline{e}(n_s)$, since the number of stationary configurations is maximal for $\alpha_+=\alpha_-=(1-n_s)/2$. This yields for the effective field $H_{\rm eff}(\alpha_+=(1-n_s)/2,\alpha_0=n_s)\equiv 0$ 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

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

The reader should note that (i) the inverse function $n_s(\overline{e})$ (see Fig. 6) of $\overline{e}(n_s)$ turns to zero at $\overline{e}=-1/4$ which equals the lowest energy of the on-site potential, but is above the ground state energy $v_0(\mu)$ and (ii) $\overline{e}(n_s)$ is not the inverse of $\overline{n_s}(e)$. 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. 3(b)]. As discussed in Appendix B, $s(e,n_s)$ has always a maximum at $\overline{n_s}(e)$ as function of n_s within its domain. $\overline{n_s}(e)$ is shown in Fig. 3(b). The

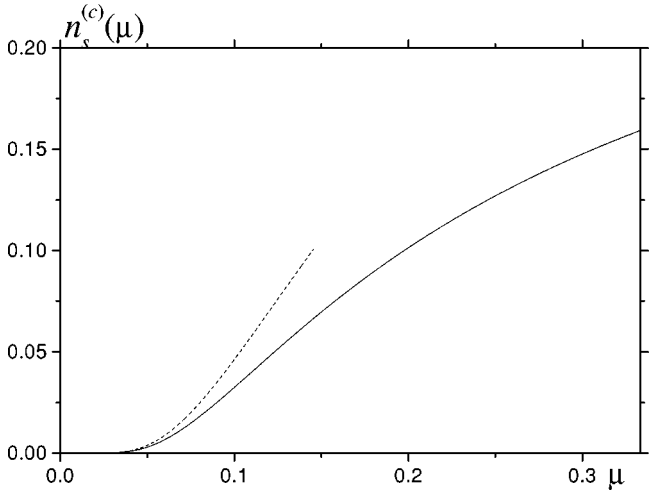

FIG. 4. μ-dependence of the critical average saddle index $n_s^{(c)}\times(\mu)$ for $0\leqslant\mu\leqslant 1/3$ (solid line). The dashed line is the asymptotic result Eq. (B5) for $\mu\ll 1$.

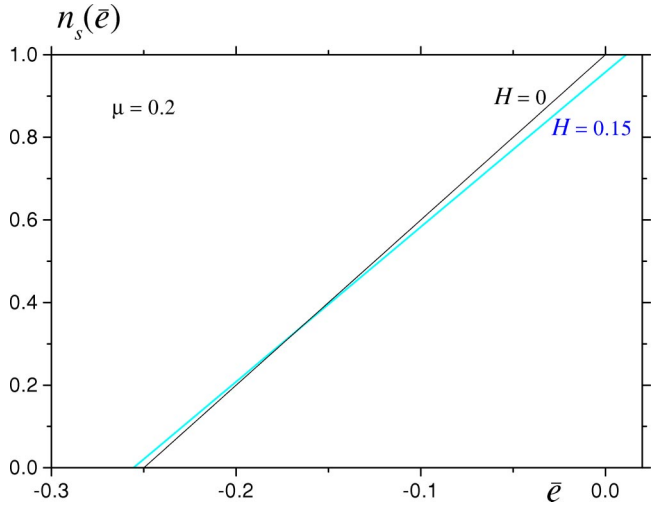

FIG. 5. Saddle index $n_s(\overline{e})$ versus averaged energy $\overline{e}$ for $\mu=0.2$ and $H=0$ and 0.15.

nonsingular e-dependence for $H\neq 0$ can clearly be seen. The average energy $\overline{e}(n_s)$ or its inverse $n_s(\overline{e})$ can be derived analytically (see Appendix B). The result for $n_s(\overline{e})$ is shown in Fig. 5.

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

$$s(e)=s(e,\overline{n_s}(e)). \tag{36}$$

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

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. (1) satisfies

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

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 $v_{\max}(\alpha_0)<e$. In this case it is independent of the energy and has the form

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

similar to Eq. (24). Hence there are two different contributions into $\chi(e)$. It can be easily shown that the contribution from the range $v_{\min}(\alpha_0)<e<v_{\max}(\alpha_0)$ for $N\to\infty$ coincides with that of $p(e)\sim\exp[Ns(e)]$ that was studied above up to an irrelevant prefactor, in spite of the sign alternation in Eq. (1). In contrast, the contribution from the range of N_s determined by $v_{\max}(\alpha_0)<e$ 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 $v_{\max}(N_s/N)=e$. One can easily see that this contribution to $\chi(e)$ never exceeds that from the range $v_{\min}(\alpha_0)<e<v_{\max}(\alpha_0)$, thus one obtains $|\chi(e)|\sim p(e)$ for $N\to\infty$.

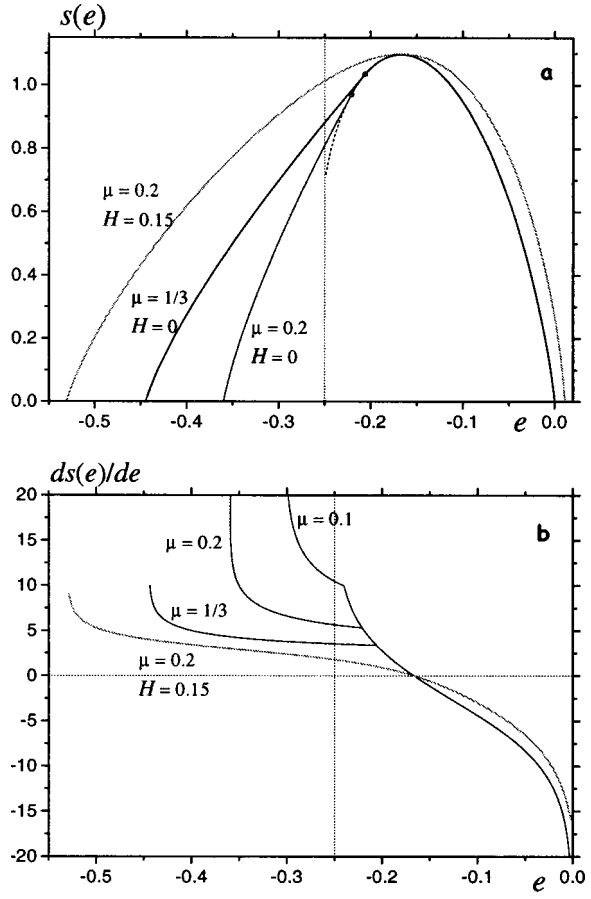

FIG. 6. (a) Energy dependence of the configurational entropy $s(e)$ for different interaction strength μ, with and without field. Dashed line is the solution for $\mu=0$ and $H=0$ and the circle indicates the location of $e_c(\mu)$; (b) Derivative of the configurational entropy showing a transition at $e=e_c(\mu)$ for $H=0$.

The reason for such peculiar behavior of the contribution from the region $v_{\max}(\alpha_0)<e$ 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,

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

This result is exact and it has a transparent topological meaning. Replacing the sum by the maximal summand value $M(N/3)$ would be an error. Even simplifying Eq. (38) with the help of the Stirling formula for $N\gg 1$ in the sum would lead to an exponentially large result instead of 1. Therefore, one should be cautious in applying the saddle point method to the right-hand side of Eq. (1).

IV. DISCUSSION

We have investigated the statistics of stationary points and topological properties of the analytically tractable potential energy surface of a ϕ^4 model in a symmetry-breaking field H with interaction of all pairs of particles with the same strength μ. For this model the mean-field approximation becomes exact in the thermodynamic limit $N\to\infty$. For $H=0$ there is a second-order phase transition at the critical temperature $T_c(\mu)$ that is analytical in μ.

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 $n_s=n_s^{\max}=1/3$. 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 $(\sigma_1,\ldots,\sigma_n)$ 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 $n_s^{\max}=1/3$ for small clusters and for liquids. We have also argued that the value $n_s^{\max}=1/3$ is a topological invariant for an entire family of ϕ^4 models. In any case, it would be important to determine $n_s^{\max}$ for other, e.g., liquidlike models and to check whether it equals again $n_s^{\max}=1/3$.

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. (37). 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. (B5). $e_c(\mu)$ is nonanalytic in μ. 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. [10–13]. 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 [10–13], 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 temperarure $T_c(\mu)$.

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 given $0<\varepsilon(\mu)<1$. If μ is small enough, which implies that the internal field is small enough, then the three roots of Eq. (15) 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 thermodynamic 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-type Hamiltonian $\mathcal{H}(\{\sigma_i\})$ (for $\mu<1/3$) with $\sigma_i=+,0,-$. The corresponding canonical partition function $\mathcal{Z}(T)=\mathrm{Tr}\exp[-\mathcal{H}(\{\sigma_i\})]$ can be calculated from the density of states $p(e)$ as

$$\mathcal{Z}(T)=\int de\, p(e)\exp[-Ne/T]. \tag{39}$$

Evidently a singularity of $\mathcal{Z}(T)$ at the corresponding transition temperature T_c' results from the underlying singularity of $p(e)$ at e_c. Obviously in this case $v_c'(\mu)=\langle\mathcal{H}\rangle(T_c')/N=e_c(\mu)$ 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 (16) satisfies $H_{\mathrm{eff}}=0$. However, for $e<e_c(\mu)$ it is $\alpha_+\neq\alpha_-$ and hence $H_{\mathrm{eff}}\neq 0$. Therefore, a spontaneous symmetry breaking occurs at both singularities.

The energy or temperature dependence of the averaged saddle index $\overline{n_s}$ seems to play a role for the dynamical features of supercooled liquids. For the present model we have found that $\overline{n_s}(e)$ vanishes at the ground state energy v_0, only. This is consistent with recent results on $\overline{n_s}(T)$ showing that $\overline{n_s}=0$ at $T=0$, only [13]. 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 $\overline{e}(n_s)$ as a function of n_s is *not* the inverse function of $\overline{n_s}(e)$. In particular $n_s(\overline{e})$ vanishes at $e^*(H)>v_0$. 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 [28], 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. III,

the first and second derivatives of $v(\alpha_+,\alpha_0)$ with respect to α_+ will be useful. A straightforward calculation making use of Eqs. (15), (16), and (20) yields

$$\frac{\partial v(\alpha_+,\alpha_0)}{\partial \alpha_+} = V_0(x_+(H_{\rm eff}),H_{\rm eff}) - V_0(x_+(H_{\rm eff}),H_{\rm eff}). \tag{A1}$$

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

$$\frac{\partial^2 v(\alpha_+,\alpha_0)}{\partial \alpha_+^2} = -[x_+(H_{\rm eff}) - x_-(H_{\rm eff})]\frac{\partial H_{\rm eff}(\alpha_+,\alpha_0)}{\partial \alpha_+} \tag{A2}$$

with

$$\frac{\partial H_{\rm eff}(\alpha_+,\alpha_0)}{\partial \alpha_+} = \mu \frac{x_+(H_{\rm eff}) - x_-(H_{\rm eff})}{1-\mu\sum_\sigma \dfrac{\alpha_\sigma}{3x_\sigma^2(H_{\rm eff})-1}}. \tag{A3}$$

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

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

$$x_-(H_{\rm eff}) \cong -1 + H_{\rm eff}/2,$$

$$x_0(H_{\rm eff}) \cong -H_{\rm eff},$$

$$x_+(H_{\rm eff}) \cong 1 + H_{\rm eff}/2 \tag{A4}$$

near $H_{\rm eff}=0$. The result is a parabola in α_+,

$$\tilde v(\alpha_+,\alpha_0) \cong -\tfrac{1}{4}(1-\alpha_0) + \frac{H^2}{2\mu} - \frac{1}{2\mu}\frac{[H+\mu(2\alpha_+ + \alpha_0 - 1)]^2}{1-\mu(1-3\alpha_0)/2}. \tag{A5}$$

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

$$\tilde v_0(\mu) = \tilde v(0,0) = -\frac{1}{4}\left(1 + \frac{2\mu}{1-\mu/2}\right),$$

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

$$v_0(\mu) = v(1,0) = v(0,0) = -\tfrac{1}{4}(1+\mu)^2, \tag{A6}$$

up to the terms μ^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

$$v_{\max}(\alpha_0) = -\frac{1}{4}(1-\alpha_0) + \frac{H^2}{2\mu}. \tag{A7}$$

The corresponding exact value of α_+ is

$$\alpha_+^{(\max)}(\alpha_0) = \frac{1-\alpha_0}{2} - \frac{H}{2\mu}. \tag{A8}$$

Equations (A7) and (A8) are thus valid for $|H| \leqslant \mu(1-\alpha_0)$.

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. (A5). Then Eq. (29) becomes quadratic, and one obtains two solutions

$$\alpha_+^{(\pm)} = \alpha_+^{(\max)}(\alpha_0) \pm \sqrt{\frac{[v_{\max}(\alpha_0) - e][1-\mu(1-3\alpha_0)/2]}{2\mu}}, \tag{B1}$$

where $\alpha_+^{(\max)}(\alpha_0)$ and $v_{\max}(\alpha_0)$ are given by Eqs. (A8) and (A7), respectively. Note that this result becomes exact for all μ with $0<\mu\leqslant 1/3$ provided that e is close to $v_{\max}(\alpha_0)$.

The density of stationary points $p(e,n_s)$ can be used to calculate the statistics of saddle indices, see Eqs. (4)–(6). The value of $\overline{n_s}(e)$ that maximizes the entropy $s(e,\alpha_0)$ on α_0 is the solution of the equation

$$\frac{\partial \alpha_+^{(+)}}{\partial \alpha_0}\ln\frac{1-\alpha_0-\alpha_+^{(+)}}{\alpha_+^{(+)}} + \ln\frac{1-\alpha_0-\alpha_+^{(+)}}{\alpha_0} = 0 \tag{B2}$$

for α_0, if this solution exists in the interval of Eq. (32). Otherwise the maximum of $s(e,\alpha_0)$ is attained at the left boundary of the α_0 window, $\alpha_0=\alpha_0^{(\min)}(e)$ [see Fig. 2(a)]. The latter solution exists only for $H=0$. It corresponds to the maxima of the curves $v(\alpha_+,\alpha_0)$ in Fig. 1(a), i.e., to

$$\alpha_+^{(+)} = \alpha_+^{(-)} = \alpha_+^{(\max)}(\alpha_0) = \frac{1-\alpha_0}{2}. \tag{B3}$$

One can see from Eq. (B1) that $\partial\alpha_+^{(+)}/\partial\alpha_0$ diverges for $e \to v_{\max}(\alpha_0)$, i.e., for $\alpha_0 \to \alpha_0^{(\min)}(e)$. 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 left-hand side of Eq. (B2) diverges at $\alpha_0 \to \alpha_0^{(\min)}(e)$, thus Eq. (B2) always has a solution, see Fig. 2(b).

Let us consider the case $H=0$ and find the condition that the solution of Eq. (B2) is just $\alpha_0=\alpha_0^{(\min)}(e)$. Simplifying this equation for $e \to v_{\max}(\alpha_0)$ one obtains the transcedental 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. 4 and the corresponding energy $e^{(c)}(\mu)$ are critical parameters that define the boundary between different regimes. In particular, $\alpha_0^{(c)}(1/3) \simeq 0.1774$ and $e^{(c)}(1/3) \simeq -0.2056$. For $\mu \ll 1$ one can solve Eq. (B4) analytically,

$$n_s^{(c)}(\mu) \equiv \alpha_0^{(c)}(\mu) \cong \frac{1}{2}\exp\left(-\frac{1}{4\mu}\right),$$

$$e_c(\mu) = -\frac{1-n_s^{(c)}(\mu)}{4} \cong -\frac{1}{4} + \frac{1}{8}\exp\left(-\frac{1}{4\mu}\right). \quad \text{(B5)}$$

Note that $e^{(c)}(\mu)$ is always above $-1/4$, the ground-state energy without interaction. Now one can write down the combined expression for $\overline{n_s}(e)$ in the case $H=0$,

$$\overline{n_s}(e) = \begin{cases} \overline{n_s^<}(e), & \upsilon_0(\mu) \leqslant e \leqslant e_c(\mu), \\ \overline{n_s^{\max}}(e), & e_c(\mu) \leqslant e \leqslant 0, \\ 0, & 0 \leqslant e. \end{cases} \quad \text{(B6)}$$

Here $\upsilon_0(\mu)$ is the ground-state energy, $\overline{n_s^<}(e)$ is equal to α_0 that solves Eq. (B2), and

$$\overline{n_s^{\max}}(e) = 1 + 4e. \quad \text{(B7)}$$

Note that the high-energy branch $\overline{n_s^{\max}}(e)$ is independent of μ and is thus the same as for a system of noninteracting particles. This contribution is due to the maxima of $\upsilon(\alpha_+, \alpha_0)$ [see Eq. (B3)] whereas $\overline{n_s^<}(e)$ is the contribution from the energy levels below this maximum. One can show that $\overline{n_s}(e) \to 0$ for $e \to \upsilon_0(\mu)$. This dependence has the form given by Eq. (34). However this dependence is only realized for the energies very close to the ground state $\upsilon_0(\mu)$. The function $\overline{n_s}(e)$ 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 $\overline{e}(n_s)$ for a given n_s. From the second of Eqs. (6) one obtains

$$\ln\frac{1-\alpha_0-\alpha_+^{(+)}}{\alpha_+^{(+)}} = 0,$$

which is simpler than Eq. (B2). From its solution

$$\overline{e}(n_s) = -\frac{1-n_s}{4} - \frac{H^2}{4}\frac{1-3n_s}{1-\mu(1-3n_s)/2} \quad \text{(B8)}$$

one obtains $n_s(\overline{e})$ shown in Fig. 5 that is almost linear in $\overline{e}$ in the considered range of parameters, Eq. (22). Note that, in contrast to $\overline{n_s}(e)$, the quantity $n_s(\overline{e})$ found from Eq. (B8) turns to zero not at the ground-state energy but at $\overline{e}=-1/4 - H^2/[2(2-\mu)]$.

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