Stability of solutions of the Sherrington-Kirkpatrick model with respect to replications of the phase space

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(Received 11 November 2004; published 3 June 2005)

We use real replicas within the Thouless, Anderson, and Palmer construction to investigate stability of solutions with respect to uniform scalings in the phase space of the Sherrington-Kirkpatrick model. We show that the demand of homogeneity of thermodynamic potentials leads in a natural way to a thermodynamically dependent ultrametric hierarchy of order parameters. The derived hierarchical mean-field equations appear equivalent to the discrete Parisi RSB scheme. The number of hierarchical levels in the construction is fixed by the global thermodynamic homogeneity expressed as generalized de Almeida-Thouless conditions. A physical interpretation of a hierarchical structure of the order parameters is gained.

DOI: 10.1103/PhysRevB.71.214403 PACS number(s): 75.50.Lk

I. INTRODUCTION

The mean-field model for spin glasses introduced by Sherrington and Kirkpatrick[1] is a paragon for complex statistical systems. Although very simple in its formulation, the model offers almost inconceivable richness of the phase space of its solution(s). This richness is manifested in the replica-symmetry breaking (RSB) solution introduced by Parisi within the replica trick.[2] Since then, a lot of supporting arguments reaching from numerical simulations[3] over analytic thermodynamic approaches without the replica trick[4] to rigorous mathematical constructions[5] have been accumulated in favor of accuracy and exactness of the Parisi RSB solution of the Sherrington-Kirkpatrick (SK) model. In spite of the amassed evidence indicating to the RSB character of the eventual solution of the SK model, we have not yet fully understood in physical terms the origin of the RSB ansatz with its ultrametric hierarchical structure of order parameters.

The replica-symmetry-breaking solution of Parisi was proposed as a means for *maximization* of the averaged free energy as a functional of the averaged order parameters in the limit of zero number of mathematical replicas. Analytic continuation from integer to noninteger numbers of replicas less than one is, however, not trivial and unique. The maximum principle seems to provide a way how to single out a particular analytic continuation. Although the Parisi ansatz provides an internally consistent solution numerically reproducing the results from Monte Carlo simulations,[6] it is not evident whether it leads to the absolute maximum of the free energy. Moreover, even when observed empirically on simpler solutions of the SK model that more stable solutions have higher averaged free energy, there is no general physical law from which we could derive the maximum principle for the averaged free energy. On the other hand, a supremum from all possible choices of the Parisi order parameters $q(x)$, $x \in [0,1]$ was proved to lead to an exact averaged free energy of the SK model.[7] The RSB scheme hence has a deeper meaning and there must be a fundamental physical principle from which one could derive the RSB solution without additional physically unjustified ansatzes.

The aim of this paper is to demonstrate that the maximum principle in the Parisi solution can be replaced by minimization of inhomogeneity of thermodynamic potentials in a successive way toward a globally thermodynamically homogeneous solution. Thermodynamic homogeneity is a fundamental property needed for the existence of a unique thermodynamic limit of statistical systems. It is a consequence of scale invariance of the limit of volume V of the system to infinity. That is, large volumes V and αV of thermodynamically homogeneous systems must produce the same thermodynamics, i.e., the same densities of extensive thermodynamic variables. Only in thermodynamically homogeneous systems the thermodynamic limit does not depend on the shape and the boundary conditions of large finite volumes.

We find it useful to apply specific scalings of extensive variables of mean-field, long-range models represented by replications of the phase space. We employ real replicas of the spin variables and demand that the thermodynamics in the replicated phase space be independent of the number of introduced equivalent replicas. The independence of the resulting averaged free energy density on the number of real replicas is investigated by studying stability of thermodynamic potentials with respect to perturbations induced by infinitesimal homogeneous interactions between different replicas. Thermodynamic potentials are stable if linear response to the interparticle interaction remains finite and the spin replicas decouple in the equilibrium state after switching off the external inter-replica interaction.

The role of real replicas in this approach is similar to the role of mathematical replicas in the replica trick. They are used to represent integer powers of the partition sum. Unlike the replica trick the number of real replicas will not be limited to zero. Alike the replica trick we will need to continue analytically the averaged replicated free energy from integer numbers of real replicas to arbitrary positive numbers to test thermodynamic homogeneity locally. For this purpose we will need to assume a symmetry of the averaged replica-dependent order parameters, Legendre conjugates to the inter-replica interaction. To find a physical motivation for a selection of a particular symmetry, we use the thermody-

namic approach of Thouless, Anderson, and Palmer (TAP). In this approach we are endowed with a set of thermodynamic mean-field parameters, local magnetizations m_i. They are supposed to determine equilibrium thermodynamic states at fixed configurations of spin-spin couplings. If the full set $m_i, i=1,\ldots,N$ determines the thermodynamic state uniquely, the replica symmetric ansatz applies as in the high-temperature phase. If not and the set of local magnetizations does not contain full information about equilibrium states, the system is thermodynamically inhomogeneous and further knowledge of the system is needed. We propose in this paper a systematic way how to retrieve the missing information about the structure of degenerate states described by a set of local magnetizations. Our construction leads in a rather direct way to an ultrametric structure of the order parameters in the (real) replica indices and to a hierarchical averaged free energy equivalent to the discrete RSB solution of Parisi.

II. THERMODYNAMIC HOMOGENEITY AND AVERAGING OF REPLICATED TAP FREE ENERGIES

A. Thermodynamic homogeneity and replications of the phase space

Homogeneity of thermodynamic potentials is one of basic principles of statistical mechanics. Thermodynamic homogeneity in systems with short-range interactions is usually expressed as the Euler condition for thermodynamic potentials (free energy) $\alpha F(T,V,N,\ldots,X_i,\ldots) = F(T,\alpha V,\alpha N,\ldots,\alpha X_i,\ldots)$, where α is an arbitrary positive number and X_i exhaust all extensive variables. Only if the Euler homogeneity is fulfilled we are able to factorize the volume from extensive variables, come over to densities, and define the thermodynamic limit uniquely and independently of the shape and boundary conditions of finite volumes. Thermodynamic homogeneity can be rephrased as a scale invariance of entropy $S(E)=k_B \ln \Gamma(E)=k_B/\nu \ln \Gamma(E)^\nu$ for arbitrary positive ν. This definition extends also to mean-field (long-range) models. We hence use the latter form of thermodynamic homogeneity applied to the averaged free energy of the SK model.

Assuming thermodynamic homogeneity we can write the averaged free energy as $F=-1/\beta\nu\langle \ln(\mathrm{Tr}\, e^{-\beta H})^\nu\rangle_{\mathrm{av}}$. If the scaling factor ν is a positive integer we can equivalently represent the discrete multiplication of the phase space via replicating the dynamical variables in the partition sum (folding of the phase space), $[\mathrm{Tr}\exp(-\beta H)]^\nu = \mathrm{Tr}_\nu \exp(\Sigma_{a=1}^{\nu}\Sigma_{\langle ij\rangle} J_{ij} S_i^a S_j^a)$. Each replicated spin variable S_i^a is treated independently, i.e., the trace operator Tr_ν operates on the ν-times replicated phase space. Calculation of the free energy in the expanded phase space amounts to evaluation of the free energy of the replicated Hamiltonian. This multiplication of the number of dynamical variables is called real replicas and has been occasionally used, mostly to illustrate the meaning of the overlap order parameters in the Parisi RSB construction.[8–10] Note that replicating the phase variables ν times is not the same operation in long-range models as a scaling of the volume $V\to\alpha V$. The spin-spin couplings, that are in short-range models intensive variables, depend in long-range models on the volume as well and are to be scaled, in the SK model as $J_{ij}\to J_{ij}/\sqrt{\alpha}$, to compensate for additional couplings in the inflated volume. Replicating of the phase space seems a more suitable and simpler tool for investigating thermodynamic homogeneity of mean-field models than direct scalings of the phase space with all new spins coupled to the old ones. When we replicate the original phase space we completely decouple the new replicated spins from the original ones and do not thereby change the normalization of the spin-spin couplings. Moreover, replication of phase variables is more suitable for investigating stability with respect to perturbations induced by interactions between different replicas without breaking translational invariance.

Real replicas are also of principal importance for the thermodynamic construction of a mean-field theory of spin glasses, since they offer a space for new symmetry-breaking fields. The real replicas are independent when introduced. We break their independence by switching on a (homogeneous) infinitesimal interaction between the replicas that we denote μ^{ab}. We then add a small interacting part $\Delta H(\mu) = \Sigma_i \Sigma_{a<b} \mu^{ab} S_i^a S_i^b$ to the replicated spin Hamiltonian. The averaged free energy per replica of the system with weakly interacting replicas reads

$$F_\nu(\mu) = -k_B T \frac{1}{\nu} \left\langle \ln \mathrm{Tr} \exp\left(-\beta \sum_\alpha H^\alpha - \beta \Delta H(\mu) \right) \right\rangle_{\mathrm{av}} . \tag{1}$$

The inter-replica interactions $\mu^{ab}>0$ play the role of symmetry-breaking fields in the SK model. They induce new order parameters in the response of the system to this field that need not vanish in the low-temperature phase, when the linear response theory breaks down. They allow to disclose the degeneracy when mean-field solutions do not represent unique pure equilibrium states. The inter-replica interactions are unphysical (not measurable) and hence to restore the physical situation we must switch off these fields at the end. If the system is homogeneous we must end up with an identity

$$\frac{d}{d\nu} \lim_{\mu\to 0} F_\nu(\mu) \equiv 0. \tag{2}$$

This quantification of thermodynamic homogeneity, thermodynamic independence of the scaling parameter ν, will lead us in the construction of a stable solution of the SK model.

B. Averaging of the replicated TAP free energy

Thermodynamic homogeneity can be investigated in the SK model either in the replica trick or in the thermodynamic TAP approach. Thermodynamic homogeneity in the replica trick is equivalent to scale invariance of the limit of the number of mathematical replicas to zero, i.e., the result should be invariant with respect to scalings of the replica index $n \to \alpha n$.[11] We prefer to use here the thermodynamic TAP approach so that to demonstrate that the RSB scheme is neither part of the replica trick nor a consequence of the limit of the number of mathematical replicas to zero. We also find the TAP approach more appropriate for finding a physical inter-

pretation of the role of the replicated spins. They are used to lift degeneracy in the determination of equilibrium thermodynamic states from the mean-field local magnetizations.

The TAP free energy can suitably be represented as

$$F = \sum_i m_i \eta_i - \frac{1}{4}\sum_{i,j} \beta J_{ij}^2 (1 - m_i^2)(1 - m_j^2) - \frac{1}{2}\sum_{i,j} J_{ij} m_i m_j - \frac{1}{\beta}\sum_i \ln 2 \cosh[\beta(h + \eta_i)]. \quad (3)$$

We introduced fluctuating internal magnetic fields η_i as variational parameters making free energy (3) together with the local magnetizations m_i extremal. The stationarity equations for the internal magnetic fields and for the local magnetizations read $\eta_i = \Sigma_j J_{ij} m_j - m_i \Sigma_j \beta J_{ij}^2 (1 - m_j^2)$, $m_i = \tanh[\beta(h + \eta_i)]$, respectively. We can now try to solve these TAP equations for m_i, η_i on finite lattices with fixed configurations of spin-spin couplings J_{ij}. We are then confronted with a plethora of metastable solutions that are difficult to handle. Instead of individual solutions we can better deal with the so-called complexity of the TAP equations, being proportional to the total number of solutions.[12]

The existence of many metastable solutions of the TAP equations generally hinders direct averaging over the random configurations of the spin-spin couplings. If the direct method is used, that is if we remain within the linear response theory with the fluctuation-dissipation theorem valid, we end up with the SK solution.[13,14] Mézard *et al.*[15] proposed the so-called cavity method to include ensembles of statistically weighted TAP solutions into the averaging process and succeeded in going beyond the SK solution toward the Parisi RSB scheme.

In this paper we want to avoid any special ansatzes about the structure or the distribution of the TAP solutions and to remain entirely within the direct averaging scheme with the ergodic and fluctuation-dissipation theorems obeyed. The fluctuation-dissipation theorem, expressed in the TAP construction as $\chi_{ii} = (1 - m_i^2)/T$, strictly holds only if the individual TAP solutions determine unique thermodynamic states. It was shown by Plefka that this is the case if $1 \geqslant \beta^2 (1 - 2\langle m_i^2 \rangle_{\mathrm{av}} + \langle m_i^4 \rangle_{\mathrm{av}})$.[16] We, however, know that this condition is violated in the low-temperature phase, which led Plefka to modifications of the TAP equations.[17]

We in principle follow an analogous way to Plefka and assume that local magnetizations determined from the TAP equations do not contain exhaustive information about the equilibrium thermodynamic states. We modify the TAP equations and connect violation of the Plefka condition with violation of thermodynamic homogeneity. We introduce real replicas into the TAP approach to substantiate this. We use the TAP free energy with ν equivalent spin replicas on each site. Real replicas were introduced into the TAP approach from a different motivation by the author years ago.[18] The result, a generalized TAP free energy with ν replicas with switched off inter-replica interactions, $\mu^{ab} = 0$, can then be overtaken from Ref. 18. It reads

$$F_\nu = \frac{1}{\nu}\sum_{a=1}^{\nu} \left[\sum_i m_i^a \left(\eta_i^a + \beta J^2 \sum_{b=1}^{a-1} \chi^{ab} m_i^b \right) + \frac{\beta J^2 N}{2} \sum_{b=1}^{a-1} (\chi^{ab})^2 - \frac{1}{4}\sum_{i,j} \beta J_{ij}^2 [1 - (m_i^a)^2][1 - (m_j^a)^2] - \frac{1}{2}\sum_{i,j} J_{ij} m_i^a m_j^a \right] - \frac{1}{\beta\nu}\sum_i \ln \mathrm{Tr} \exp\left(\beta^2 J^2 \sum_{a<b}^{\nu} \chi^{ab} S_i^a S_i^b + \beta \sum_{a=1}^{\nu} (h + \eta_i^a) S_i^a \right). \quad (4)$$

Here m_i^a are local magnetizations and η_i^a are local internal magnetic fields. They are configurationally dependent variational variables determined from stationarity equations. Parameters χ^{ab}, $a \neq b$, are overlap susceptibilities and are global (translationally invariant) variational variables, Legendre conjugates to the symmetry breaking fields μ^{ab}. They are the genuine order parameters in the spin glass phase of the SK model in this construction. At the saddle point we have $\chi^{ab} = N^{-1}\Sigma_i (\langle S_i^a S_i^b \rangle_T - \langle S_i^a \rangle_T \langle S_i^b \rangle_T)$.

Free energy F_ν from Eq. (4) is averaged over thermal fluctuations for one configuration of spin-spin couplings J_{ij}. To perform averaging over the randomness in the spin-spin couplings we must decide whether the solutions of the replicated TAP equations, stationarity equations derived from free energy (4), determine unique equilibrium thermodynamic states or not. If not, we must surmise the internal structure of equilibrium states represented by a set of local magnetizations and averaged overlap susceptibilities. It can be done only via an ansatz. The pure states in spin glasses are, however, peculiar in that respect that they cannot be singled out by external symmetry-breaking fields. To avoid application of any unjustified ansatzes, we assume that the solutions of the replicated TAP equations do represent unique thermodynamic states as it is the case in the high-temperature phase. It means that replication of the phase space serves as a replacement of symmetry breaking fields. Replicating the phase space enables us to extend the high-temperature properties, that is the replica symmetric ansatz, to low temperatures in analogy to the ferromagnet in an external magnetic field. Then the linear response, ergodic and fluctuation-dissipation theorems hold and we can use the same averaging of the replicated TAP free energy as used to derive the SK solution from the TAP free energy.

Even with the assumption of uniqueness of equilibrium states in the replicated phase space the averaging of the replicated free energy (4) cannot be performed explicitly. We first must quantify thermodynamic equivalence of the replicated spin variables. Since the replicated spin variables were introduced in the TAP approach to deal with a possible degeneracy of solutions of the TAP equations properly, we assume the following thermodynamic equivalence of real replicas motivated by the paramagnetic solution:

$$m_i^a \equiv \langle S_i^a \rangle_T = m_i. \quad (5)$$

There is no apparent reason for breaking this equivalence in the spin glass phase, since each copy of the spin variables shares the same external macroscopic parameters determining the thermodynamic state. Equation (5) expresses the fact

that each TAP solution with local magnetizations m_i represents on average ν thermodynamic states labeled by the replica index a. The different thermodynamic states are indistinguishable at the level of local magnetizations. Since the replicated spin variables are distinct, their local overlap susceptibility is not, however, determined from the fluctuation-dissipation theorem and enters the free energy as a variational parameter. Equivalence of spin replicas, Eq. (5), leads then to independence of local magnetic fields η_i^a and the sum of the averaged overlap susceptibilities $\Sigma_b \chi^{ab}$ of the replica index a. With this conclusion we can write down an explicit representation of the averaged free energy density with ν equivalent real replicas

$$f_\nu = \frac{\beta J^2}{4}\left(\frac{1}{\nu}\sum_{a\neq b}^{\nu}[(\chi^{ab})^2 + 2q\chi^{ab}] - (1-q)^2\right) - \frac{1}{\beta\nu}\int_{-\infty}^{\infty}\frac{d\eta}{\sqrt{2\pi}}e^{-\eta^2/2}\ln \mathrm{Tr}\exp\left(\beta^2 J^2\sum_{a<b}^{\nu}\chi^{ab}S^aS^b + \beta\bar{h}\sum_{a=1}^{\nu}S^a\right). \tag{6}$$

We denoted the fluctuating magnetic field $\bar{h}=h+\eta\sqrt{q}$. The averaged order parameters are at the saddle point $q=\langle\langle S^a\rangle_T^2\rangle_{\mathrm{av}}$ and $\chi^{ab}=\langle\langle S^aS^b\rangle_T\rangle_{\mathrm{av}}-q$.

The trace in the averaged free energy density (6) cannot be evaluated explicitly. To do so we must know the matrix of the overlap susceptibilities χ^{ab} reflecting the structure of thermodynamic states indistinguishable in the TAP equations. Mathematically it means to find the most general structure of matrix χ^{ab} with the constraint that $\Sigma_b\chi^{ab}$ does not depend on a. Since we do not know how such a structure should look, we must make a choice and check only *a posteriori*, whether our choice has led to a consistent solution. We use an iterative construction with successive replications of the phase space accompanied by the replica-symmetric ansatz for the overlap susceptibilities at each step. We replicate the system so many times until a thermodynamically homogeneous solution satisfying Eq. (2) is reached.

C. Analytic continuation and local and global thermodynamic homogeneity

The mean-field (saddle-point) equations for χ^{ab} derived from the averaged free energy density (6) are identical for all pairs of the replica indices $(ab), a\neq b$. There is no apparent symmetry breaking force in the replica space and $\chi^{ab}=\chi$ is evidently a possible solution. We choose this simplest, replica-symmetric solution so that we can evaluate the averaged free energy explicitly. This replica-symmetric choice corresponds physically to a situation where the TAP solutions comprise of equivalent distinguishable thermodynamic states with the same overlap susceptibility (distance) between each pair of different states. Hence no internal structure of equilibrium states is assumed.

It is straightforward to evaluate the averaged free energy density f_ν with the ansatz $\chi^{ab}=\chi$. We employ the Hubbard-Stratonovich transformation to decouple the replicated spins and end up with

$$f_\nu(q,\chi) = -\frac{\beta}{4}(1-q)^2 + \frac{\beta}{4}(\nu-1)\chi(2q+\chi) + \frac{\beta}{2}\chi - \frac{1}{\beta\nu}\int_{-\infty}^{\infty}\mathcal{D}\eta\ln\int_{-\infty}^{\infty}\mathcal{D}\lambda\{2\cosh[\beta(h+\eta\sqrt{q}+\lambda\sqrt{\chi})]\}^\nu, \tag{7}$$

where we used an abbreviation for the Gaussian differential $\mathcal{D}\phi\equiv d\phi e^{-\phi^2/2}/\sqrt{2\pi}$. We set $J=1$ and use this energy scale throughout the rest of the paper.

The averaged free energy density, Eq. (7), however, apparently depends on ν whenever the order parameter $\chi>0$. It is the case in the spin-glass phase below the de Almeida-Thouless (AT) instability line. Free energy (7) has the form identical with the Parisi one-step RSB solution, where ν plays the role of the parameter dividing the replica space in the RSB ansatz.[2] We can easily analytically continue the right-hand side (rhs) of Eq. (7) to all real numbers. The integral representation in Eq. (7) is well defined and analytic for $\nu\in(-\infty,\infty)$.

There are two observations we can make from the analysis of free energy (7). First, at any value of ν the overlap susceptibility is positive below the AT line. It indicates that the SK solution ($\chi=0$) becomes thermodynamically inhomogeneous. Second, we are unable to find parameters q,χ for which free energy (7) would be ν independent and hence the TAP solutions indeed do not describe unique thermodynamic states in the low-temperature phase. Our modification of the TAP free energy becomes nontrivial.

Free energy (7) is not globally thermodynamically homogeneous, since it depends on the scaling parameter ν. We can, however, optimize the solution in that we demand that the deviations from the thermodynamic homogeneity be minimal. This is achieved if at least thermodynamic homogeneity is obeyed locally, that is, if

$$\frac{\partial f_\nu(q,\chi)}{\partial\nu} = 0. \tag{8}$$

This equation determines an optimal parameter ν_{opt} for which the free energy is locally thermodynamically homogeneous. We show later on that Eq. (8) has always a solution with $\nu_{\mathrm{opt}}>0$. Free energy (7) together with the optimization condition (8) exactly deliver the thermodynamics of the Parisi one-step RSB. Monasson and later Mézard proposed in Refs. 19 and 20 a similar approach to the thermodynamics of structural glasses, the so-called cloned liquid. The local homogeneity, Eq. (8), was interpreted there as vanishing of complexity.

Satisfying thermodynamic homogeneity locally for the optimal parameter ν_{opt} is generally insufficient. We in fact should construct a theory being globally thermodynamically homogeneous. To check whether free energy (7) can for any ν be globally thermodynamically homogeneous we must perform a further scaling of extensive variables via replicating the spin variables in Eq. (6). We do so by replacing $\nu\to n\nu$

and testing homogeneity of the free energy f_ν with respect to the n-times enlarged (replicated) phase space. With the new scaling we must replicate each spin variable S^a to $(S^\alpha)^a$ and transform the matrix of overlap susceptibilities to a super matrix $\chi^{ab} \to (\chi^{\alpha\beta})^{ab}$ where $a,b=1,\ldots,\nu$ and $\alpha,\beta=1,\ldots,n$. With this replication we allow that the local spin variables S^a may still be insufficient to determine unique thermodynamic states. Since all spin variables S^a are thermodynamically equivalent, they must split into new states labeled by the new replica index α identically.

The mean-field equations for $(\chi^{\alpha\beta})^{ab}$ again contain a replica-symmetric solution $\chi_1=(\chi^{\alpha\beta})^{ab}$ for $a\neq b$ and $\chi_2=(\chi^{\alpha\beta})^{aa}$ for $\alpha\neq\beta$. This symmetric solution assumes that the local TAP magnetization m_i can be represented by ν composite states each of which contains n pure states. Two pure states are distinguished by the overlap susceptibility χ_2 if they peel off from the same parental spin S^a and by χ_1 if they stem from two different parental spins S^a, S^b, $a\neq b$.

It follows from the presented construction that $\chi_1 \geqslant \chi_2$. The free energy now generally depends on n,ν and χ_1,χ_2. We obtain explicitly

$$f_{\nu,n}(q,\chi_1,\chi_2) = -\frac{\beta}{4}(1-q)^2 + \frac{\beta}{2}\chi_1 + \frac{\beta}{4}[(\nu-1)\chi_1(2q+\chi_1) + \nu(n-1)\chi_2(2q+\chi_2)] - \frac{1}{\beta\nu n}\int \mathcal{D}\eta \ln \int \mathcal{D}\lambda_2\left(\int \mathcal{D}\lambda_1\{2\cosh[\beta(h + \eta\sqrt{q} + \lambda_1\sqrt{\chi_1-\chi_2} + \lambda\sqrt{\chi_2})]\}^\nu\right)^n, \quad (9)$$

which again is equivalent to the Parisi 2RSB free energy. Free energy $f_{\nu,n}$ from Eq. (9) is independent of n and reduces to f_ν from Eq. (7) if and only if $\chi_2=0$.

When this "second level" free energy $f_{\nu,n}$ depends on n it can be optimized so that it is locally thermodynamically homogeneous. The result can be subject to a further scaling of extensive variables in order to verify whether the resulting thermodynamic potential is globally homogeneous. We can proceed with the hierarchical (multiplicative) scalings accompanied with the replica-symmetric ansatz about the structure of the newly generated overlap susceptibilities so long until the free energy becomes a thermodynamically homogeneous function, i.e., the free energy does not depend on the last scaling parameter. It is evident that with each transformation we generate just one scaling parameter m_l and one block-off-diagonal matrix of the overlap susceptibility χ_l.

III. HIERARCHICAL MEAN-FIELD THEORY

A. Hierarchical free energy

After performing K scaling transformations (replications of spin variables) we end up with K geometric parameters $m_1<m_2<\cdots<m_K=\nu$ as well as K overlap susceptibilities $\chi_1\geqslant\chi_2\geqslant\cdots\chi_K\geqslant 0$ characterizing the phase space of the order parameters. At each step (hierarchical level) of this construction we use the Hubbard-Stratonovich transformation to linearize the newly introduced (replicated) spin variables in free energy (6). If we define $m_0=1$ and $\chi_{K+1}=0$ we can represent the averaged free energy density with K hierarchical scaling transformations in the following form:

$$f_K(q,\{\chi\};\{m\}) = -\frac{\beta}{4}(1-q)^2 + \frac{\beta}{4}\sum_{l=1}^{K}(m_l-m_{l-1})\chi_l(2q+\chi_l) + \frac{\beta}{2}\chi_1 - \frac{1}{\beta\nu}\int_{-\infty}^{\infty}\frac{d\eta}{\sqrt{2\pi}}e^{-\eta^2/2}\ln\left[\int_{-\infty}^{\infty}\frac{d\lambda_K}{\sqrt{2\pi}}e^{-\lambda_K^2/2} \times\left(\cdots\int_{-\infty}^{\infty}\frac{d\lambda_1}{\sqrt{2\pi}}e^{-\lambda_1^2/2}\left\{2\cosh\left[\beta\left(h+\eta\sqrt{q}+\sum_{l=1}^{K}\lambda_l\sqrt{\chi_l-\chi_{l+1}}\right)\right]\right\}^{m_1}\cdots\right)^{m_K/m_{K-1}}\right]. \quad (10)$$

In this expression q and χ_l, $l=1,\ldots,K$ are physical order parameters and are determined from the saddle-point equations. The numbers m_l, $l=1,\ldots,K$ are formally external geometric parameters determining the replica-symmetry breaking scheme of the matrix χ^{ab} from Eq. (6). They parametrize successive scalings (replications) of extensive variables that would not change thermodynamically homogeneous solutions.

It is evident that the averaged free energy density (10) can be uniquely analytically continued to arbitrary non-negative numbers $m_1,\ldots,m_K=\nu$, since it is represented by analytic functions for all non-negative variables m_l, $l=1,\ldots,K$. In the analytically continued function, the geometric parameters m_l need no longer be integers and either they need not form an ascending sequence.

To find out whether a specific choice of geometric parameters m_l can lead to a thermodynamically homogeneous solution we must understand how the free energy depends on these parameters. We obtain from the structure of the rhs of Eq. (10) the following identities:

$$f_K(q,\{\chi\};\{m,m_K=m_{K-1}\}) = f_{K-1}(q,\{\chi\};\{m\}), \quad (11a)$$

$$f_K(q,\{\chi\};\{m,m_K=0\}) = f_{K-1}(q+\chi_K,\{\chi;\chi_i=\chi_i-\chi_K\};\{m\}), \quad (11b)$$

$$f_K(q,\{\chi,\chi_i=\chi_{i+1}\};\{m\}) = f_{K-1}(q,\{\chi\};\{m\}). \quad (11c)$$

The solutions in the first and third cases are degenerate. The averaged free energy density f_K does not depend on χ_K in Eq.

(11a) and it is independent of m_i in Eq. (11c). Further on, if $m_K \geqslant m_{K-1}$ then $f_K \leqslant f_{K-1}$. We hence can conclude that if f_K *does depend* on m_K, i.e., it is inhomogeneous, the averaged free energy displays a local *maximum* for some value $m_K \in (0, m_{K-1})$. Free energy $f_K(q,\{\chi\};\{m\})$ is independent of $\nu = m_K$ if and only if $\chi_K = 0$.

That is, we can find such a parameter m_K at which the averaged free energy density $f_K(q,\{\chi\};\{m\})$ reaches a local saddle point for the given values of $m_1,\ldots,m_{K-1}$ with respect to variations of the parameter m_K. Consequently, we can add the geometric parameters characterizing the structure of the phase space to the variational parameters. If the solution does not obey the global homogeneity condition $\partial f_K(q,\{\chi\};\{m\})/\partial m_K \equiv 0$, the local homogeneity condition $\partial f_K(q,\{\chi\};\{m\})/\partial m_K = 0$ then minimizes deviations from the global thermodynamic homogeneity. It immediately follows from Eqs. (11) that this stationarity point is a *local maximum*. We fix in this way any new geometric parameter emerging in the hierarchical construction and achieve a theory with a thermodynamically determined ultrametric structure. Notice, that both sets of parameters $\chi_1,\ldots,\chi_K$ and $m_1,\ldots,m_K$ form sequences of decreasing numbers from interval [0, 1]. It is easy to verify that a substitution $q^{ab} = q + \chi^{ab}$ in Eq. (10) recovers the Parisi RSB solution with K discrete hierarchies.[21]

B. Hierarchical stationarity equations

To simplify the analysis of properties of the hierarchical free energy and the stationarity equations determining the variational parameters χ_l and m_l we rewrite the rhs of Eq. (10) in a recursive way. We define a sequence of partition functions

$$Z_l = \left(\int_{-\infty}^{\infty} \mathcal{D}\lambda_l Z_{l-1}^{m_l} \right)^{1/m_l} \tag{12}$$

with the initial condition $Z_0 = \cosh[\beta(h + \eta\sqrt{q} + \Sigma_{l=1}^{K}\lambda_l\sqrt{\Delta\chi_l} + \lambda\sqrt{\Delta\chi})]$. We denoted $\Delta\chi_l = \chi_l - \chi_{l+1}$ and $\Delta\chi \equiv \chi_{K+1} = \chi - \Sigma_{l=1}^{K}\Delta\chi_l$. We singled out the scaling parameter ν from the other geometric parameters. The averaged free energy density can then alternatively be represented as

$$\begin{aligned} f_K^{\nu}(q,\chi,\Delta\chi_1,\ldots,\Delta\chi_K;m_1,\ldots,m_K) &= -\frac{\beta}{4}(1-q-\chi)^2 + \frac{\beta}{4}\nu\Delta\chi(2q+\Delta\chi) - \frac{1}{\beta}\ln 2 \\ &+ \frac{\beta}{4}\sum_{l=1}^{K} m_l \Delta\chi_l \left[2\left(q + \chi - \sum_{i=1}^{l-1}\Delta\chi_i \right) - \Delta\chi_l \right] \\ &- \frac{1}{\beta}\int_{-\infty}^{\infty} \mathcal{D}\eta \ln\left(\int_{-\infty}^{\infty} \mathcal{D}\lambda Z_K^{\nu} \right)^{1/\nu} \end{aligned} \tag{13}$$

with q, χ, $\Delta\chi_l$, $l=1,\ldots,K$ and m_l, $l=1,\ldots,K$ as order parameters to be determined from stationarity equations. The number of hierarchies K used in the free energy should be chosen so that f_K^{ν} does not depend on the scaling parameter ν.

To represent the mean-field equations we introduce a set of hierarchical density matrices in the space of fluctuating random fields λ_l. We define $\rho_l(\eta,\lambda;\lambda_K,\ldots,\lambda_l) = Z_l^{m_l}/\langle Z_l^{m_l}\rangle_{\lambda_l}$ and $\rho(\eta,\lambda) = Z^{\nu}/\langle Z^{\nu}\rangle_{\lambda}$ with $Z = \langle Z_K^{m_K}\rangle_{\lambda_K}^{1/m_k}$. We further introduce short-hand notations $t \equiv \tanh[\beta(h + \eta\sqrt{q} + \lambda\sqrt{\Delta\chi} + \Sigma_{l=1}^{K}\lambda_l\sqrt{\Delta\chi_l})]$ and $\langle t\rangle_l(\eta,\lambda;\lambda_K,\ldots,\lambda_{l+1}) = \langle \rho_l \cdots \langle \rho_1 t\rangle_{\lambda_1}\cdots\rangle_{\lambda_l}$ with $\langle X(\lambda_l)\rangle_{\lambda_l} = \int_{-\infty}^{\infty}\mathcal{D}\lambda_l X(\lambda_l)$.

With the above definitions we can write down the stationarity equations for the physical order parameters,

$$q(\nu,K) = \langle\langle \rho\langle t\rangle_K\rangle_{\lambda}^2\rangle_{\eta}, \tag{14a}$$

$$\chi(\nu,K) = \langle\langle \rho\langle t^2\rangle_K\rangle_{\lambda}\rangle_{\eta} - \langle\langle \rho\langle t\rangle_K\rangle_{\lambda}^2\rangle_{\eta}, \tag{14b}$$

$$\Delta\chi_l(\nu,K) = \langle\langle \rho\langle\langle t\rangle_{l-1}^2\rangle_K\rangle_{\lambda}\rangle_{\eta} - \langle\langle \rho\langle\langle t\rangle_l^2\rangle_K\rangle_{\lambda}\rangle_{\eta}, \tag{14c}$$

and for the geometric ones

$$m_l(\nu,K) = \frac{4}{\beta^2}\frac{\langle\langle \rho\langle \ln Z_{l-1}\rangle_K\rangle_{\lambda}\rangle_{\eta} - \langle\langle \rho\langle \ln Z_l\rangle_K\rangle_{\lambda}\rangle_{\eta}}{\langle\langle \rho\langle\langle t\rangle_{l-1}^2\rangle_K\rangle_{\lambda}\rangle_{\eta}^2 - \langle\langle \rho\langle\langle t\rangle_l^2\rangle_K\rangle_{\lambda}\rangle_{\eta}^2}, \tag{15}$$

where index $l=1,\ldots,K$. A thermodynamically homogeneous solution is obtained if $\chi = \Sigma_{l=1}^{K}\Delta\chi_l$ and the remaining $2K+1$ order parameters do not depend on ν.

C. Stability conditions

Averaged free-energy density (13) defines a solution of the SK model with K hierarchical levels labeled by a scaling parameter ν. A globally thermodynamically homogeneous averaged free energy may not depend on ν. This happens if $\chi = \Sigma_{l=1}^{K}\Delta\chi_l$. This condition of global thermodynamic homogeneity is satisfied if an inequality

$$1 \geqslant \beta^2 \left\langle \left\langle 1 - t^2 + \sum_{l=1}^{K} m_l(\langle t\rangle_{l-1}^2 - \langle t\rangle_l^2) \right\rangle_K^2 \right\rangle_{\eta} \tag{16a}$$

is fulfilled. This inequality, however, does not represent the only stability condition for a multilevel hierarchical free energy. A hierarchical solution with K levels is stable if it does not decay into a solution with $K+1$ hierarchies. A new order parameter $\Delta\chi$ may emerge so that $\Delta\chi_l > \Delta\chi > \Delta\chi_{l+1}$ for arbitrary l. That is, the new order parameter peels off from $\Delta\chi_l$ and shifts the numeration of the order parameters for $i > l$ in the existing K-level solution. To guarantee that this does not happen and that the averaged free energy depends on no more geometric parameters than $m_1,\ldots,m_K$ we must fulfill a set of K generalized AT stability criterions that for our hierarchical solution read for $l=1,2,\ldots,K-1$,

$$1 \geqslant \beta^2 \left\langle \left\langle \left\langle 1 - t^2 + \sum_{i=1}^{l} m_i(\langle t\rangle_{i-1}^2 - \langle t\rangle_i^2) \right\rangle_l^2 \right\rangle_K \right\rangle_{\eta}. \tag{16b}$$

There is also a condition that the new order parameter emerges as the largest difference, that is $\Delta\chi > \Delta\chi_1$. So that neither this instability takes place we must fulfill

$$1 \geqslant \beta^2 \langle\langle (1-t^2)^2\rangle_K\rangle_{\eta}. \tag{16c}$$

Actually, it is sufficient to take into account only a single stability condition, namely that with the maximal right-hand

side of Eqs. (16). Which of these right-hand sides is maximal depends on the particular choice of the optimal geometric parameters $m_1,\ldots,m_K$ minimizing thermodynamic inhomogeneity of the hierarchical solution with lower numbers of hierarchical levels.

D. Physical interpretation of the order parameters from the hierarchical free energy

The hierarchical free energy, Eq. (13), is equivalent to the Parisi discrete RSB solution with K hierarchies. Hence the resulting stationarity equations, Eqs. (14) and (15), coincide with the stationarity equations derived from the K-step RSB free energy when we make a substitution $q^{ab}=q+\chi^{ab}$. The derived numbers must be the same. The meaning and a physical interpretation of the order parameters in both approaches may, however, be different. Different interpretations of the role of the order parameters, in particular of the geometric ones, originate from the way the hierarchical free energy (13) was derived. The RSB free energy was derived in an effort to maximize the averaged free energy within the replica trick and the discrete scheme (13) was used as an intermediate step toward its eventual form—the limit $K\rightarrow\infty$ and continuously distributed order parameters $q(x)$, $x\in[0,1]$. The physical interpretation of the Parisi RSB solution is then based on this continuous limit.[4] The present approach does not provide justification for the continuous limit and the physical meaning of the order parameters in the hierarchical free energy must be sought within the discrete scheme.

The hierarchical free energy was derived by replica-symmetric averaging of the TAP free energy extended to a replicated phase space. Real replicas in the thermodynamic TAP approach were introduced to include control over thermodynamic homogeneity. Thermodynamic homogeneity is tightly connected with uniqueness of equilibrium states determined by mean-field local magnetizations calculated from the TAP equations. The TAP equations define a unique thermodynamic state if the solution reacts to all possible perturbations identically and no possible internal structure of the solution can be revealed. We showed that by replicating the phase space we indeed reveal an internal structure of the TAP solutions.

It is clear from the construction itself that the overlap susceptibilities χ^{ab} measure the interaction strength with which different copies of spins thermodynamically influence each other. That is, the thermal averaging of one spin copy depends on the values of spins in the other copies if $\chi^{ab}>0$. We cannot separate individual replicas although only one spin replica represents the physical system under consideration. The nonreplicated original phase variables together with temperature and the chemical potential are hence insufficient to describe entirely the equilibrium thermodynamic states. To get rid of the dependence of thermodynamic states on boundary or initial conditions we must average over all initial/boundary values and external variables that influence the thermodynamics of the investigated system. In long-range, completely connected models the degeneracy in solutions of the mean-field equations is reflected in the dependence on the initial spin configurations. We simulated this dependence in our approach with replicas of the spin variables subject to the same thermal equilibration.

If a mean-field solution is thermodynamically inhomogeneous, thermal equilibration depends on the initial spin configuration. Dependence of the thermodynamic state on the initial spin configuration from which we start equilibration may have a nontrivial form. It is reflected in our approach in the matrix χ^{ab}. The replica-symmetric ansatz, $\chi^{ab}=\chi$, means that all the initial spin configurations are equivalent and that there is only a single "mean" strength with which they affect the resulting equilibrium state. The replica symmetric ansatz is the most natural first guess motivated by the high-temperature phase but need not lead to a thermodynamically homogeneous solution. The dependence of the equilibrium states on their initial configurations should be chosen so as to reach a globally homogeneous solution. To achieve this goal we apply successive replications using only the simplest, replica-symmetric ansatz from the high-temperature solution at each stage. This construction seems to be more transparent than an unjustified replica symmetry-breaking ansatz. Moreover, the iterative construction offers an appealing physical interpretation of the geometric order parameters used in the hierarchical solution (13).

To understand the role of the geometric parameters let us first take the 1RSB free energy (7). The interacting part of the averaged TAP free energy density reads

$$-\frac{N}{\beta V}\ln Z_0(\beta,h)\rightarrow-\frac{1}{\beta\nu V}\ln\left(\int \mathcal{D}\lambda Z_0(\beta,h+\lambda\sqrt{\chi})^{\nu}\right)^{N}. \tag{17}$$

We can see that the replicated spins influence the original spins by making the internal magnetic field dynamically random. The replicated free energy then behaves as if effectively νN spins of the original system enclosed in the volume νV were affected by the replicated spins outside the system under consideration. The internal magnetic field changes due to the existence of replicated spins to $h\rightarrow h+\lambda\sqrt{\chi}$. The integral over the fluctuating variable λ stands for averaging over the replicated (external) spins. The averaging over the replicated spins is dynamical (annealed), in contrast to the quenched (static) averaging over the random configurations of the spin exchange. The parameter ν is then kind of a chemical potential governing the exchange between the active and additional replicated spin configurations. It must be chosen so as the external replicated spins minimally influenced the final equilibrium state of our original system.

Adding more geometric order parameters with $1>m_1>\cdots>m_K>0$ in the full hierarchical free energy means that the true equilibrium states are hierarchically dependent on the initial spin configurations or they depend on the history of quasiequilibrium states they went through during thermal averaging. When the thermodynamic equilibrium of the original system depends on configurations of replicated spins we must include the replicated spins into our global thermodynamic system. In this merge we compose the total number of N spins from m_1N from the original system and $(1-m_1)N$ from the replicated one. The parameter m_1 is to be

chosen so as to minimize the impact of the replicated spins on the original ones. Only the original spins, however, represent active variables, while the replicated ones form kind of a thermal bath. We must include the bath explicitly into thermal equilibration of the active spin variables, since the latter are affected by the former. The bath spins affect the thermodynamics of the active spins via the overlap susceptibility χ_1 modifying their internal magnetic field. We further replicate the N spin variables in the whole volume and test whether our m_1N active spins interacting with the bath with the overlap susceptibility χ_1 are affected by this replication. If yes, we must include the new replicated spins into thermal averaging. We denote χ_2 the strength with which the new (second level) replicas affect the internal magnetic field of the active spins. The bath spins (first level replicas) are then affected by the new spin replicas in the same way as the first-level replicas act on the active spins, that is via an overlap susceptibility $\chi_1 > \chi_2$. The optimal restructuring of spins in the whole system is such that only m_2N spins belong to the active ones, m_1N are from the first-level bath and the rest of $(1-m_1)N$ spins are the new replicated spins, second-level bath. The parameters m_1 and m_2 are dynamically determined from minimization of the impact of the newly replicated spins on the active ones. We continue with wrapping the active spin variables in successively replicated ones so long until we reach independence of the active spins on phase-space replications. The hierarchical construction converges toward a globally homogeneous solution if $\chi_1. > \chi_2 > \cdots > \chi_K \to 0$, or $\chi_{K+1}=0$ at a finite number of hierarchies K.

Alternatively we can interpret the free energy (13) as a solution with a multitude of equivalent equilibrium thermodynamic states. Each state extends on average over a portion m_KN of the whole spin space. The states are organized hierarchically with on average $(m_{K-1}-m_K)/m_K$ nearest neighbors with the overlap susceptibility χ_K, $(m_{K-2}-m_{K-1})/m_K$ next nearest neighbors with the overlap susceptibility χ_{K-1}, and so on. The last Kth level is characterized by $(1-m_1)/m_K$ neighbors with the overlap susceptibility χ_1. The total number of equilibrium states then statistically is $1/m_K$. It is clear that pure states cannot be singled out and separated from their neighbors. Only the whole complex of hierarchically arranged states can be thermodynamically homogeneous and form an independent system with a well-defined thermodynamic limit.

IV. CONCLUSIONS

We used the basic physical principle of thermodynamic homogeneity and derived with the aid of real replicas in the thermodynamic TAP approach a hierarchical representation for the averaged free energy of the SK model. The hierarchical free energy (13) was derived via successive replications of the phase space with the replica symmetric ansatz for the introduced order parameters—overlap susceptibilities. Real replicas proved to be a suitable tool for treating situations when the TAP order parameters, local magnetizations, do not describe unique thermodynamic states. Real replicas enable one to lift the degeneracy of the TAP approach and provide for a larger phase space within which a thermodynamically homogeneous solution can be found. The replica symmetric ansatz reflects an assumption of no internal structure (metric) of the thermodynamic states corresponding to a given set of local magnetizations from the TAP equations. This is the most natural (minimal) choice when we do not know the actual structure and organization of equilibrium states. Successive scalings in the phase space and the property of global thermodynamic homogeneity then lead to a selection of a nontrivial, ultrametric structure of thermodynamic states. We apply so many scalings of extensive variables (hierarchical levels) until the global thermodynamic homogeneity is achieved.

The averaged free energy (13) derived in this way is equivalent to the Parisi discrete RSB solution. It contains a set of averaged physical parameters q, χ_l, $l=1,\ldots,K$ and a set of geometric parameters m_l, $l=1,\ldots,K$. The geometric parameters are turned variational ones by the demand of local thermodynamic homogeneity at each step of the hierarchical construction. The principle of local thermodynamic homogeneity replaces the maximum principle in the Parisi RSB construction. The homogeneity is reached successively by demanding stability with respect to scalings of extensive variables. Each hierarchical level then *minimizes* deviations from the global homogeneity and hence the instability of the solution. The maximum principle of Parisi emerges as a consequence of minimization of thermodynamic inhomogeneity of intermediate solutions and the form of stationarity equations for the SK model. However, it does not mean that the absolute maximum of the averaged free energy should be the equilibrium solution. The maximum principle holds only for thermodynamically inhomogeneous states. The free energy should still be minimal among thermodynamically homogeneous states.

We were able to derive the discrete Parisi RSB scheme from a physical principle of thermodynamic homogeneity but we do not find justification for its continuous version characterized by a nonlinear differential equation. The continuous version emerges in the limit $K\to\infty$ by assuming infinitesimal smallness of the overlap susceptibilities, $\chi_l = \Delta_l/K$ and infinitesimal differences in the geometric parameters $m_l/m_{l+1}=1+\delta_l/K$. In the continuous limit of the RSB scheme the geometric parameters are no longer determined thermodynamically, they cover interval $[0, 1]$. Only an order-parameter function $q(x)$ for $x\in[0,1]$ is to be determined variationally. In the discrete scheme the geometric order parameters form a discrete set and are determined thermodynamically from Eq. (15) for $l=1,2,\ldots,K$. These equations are an essential part of the hierarchical solution and are of particular importance at low temperatures. Only with thermodynamically determined geometric parameters we are able to improve upon the SK free energy at zero temperature. At low temperatures, new variational parameters $x_l=\beta m_l$ are to be introduced and used instead of m_l. Moreover, the thermodynamically shaped ultrametric structure of equilibrium states in the discrete scheme leads to tangible nonlinear effects. They get lost in the continuous limit. To decide whether the discrete or continuous versions of the Parisi solution with $K=\infty$ holds in the SK model, one must evaluate the discrete scheme near the spin-glass transition point, which has not yet been done. Work on the comparison of

discrete and continuous versions of the RSB near the critical temperature is in progress.

Thermodynamic inhomogeneity of the SK solution in the real-replica approach was attributed to ambiguity of solutions of the TAP equations in the determination of pure equilibrium states. Although real replicas offer a way how to identify this degeneracy, they do not allow for separation of individual pure states. That is why an organization of thermodynamic states cannot be determined without an ansatz. We hence cannot find a fully ansatz-free solution of the SK model. Successive scaling transformations with the replica symmetric ansatz allow the system to arrange equilibrium states so that thermodynamic inhomogeneity at intermediate states is minimal. It recovers the Parisi discrete RSB scheme, but we cannot claim that this is the only thermodynamically homogeneous solution. At present, we cannot even prove that the full (infinite level) solution is indeed thermodynamically homogeneous, that is, it fulfills stability conditions (16). Nevertheless, the proposed construction seems to offer a rather straightforward way based on basic principles of statistical mechanics to reach the discrete RSB solution with stability conditions and an appealing physical interpretation.

To conclude, we demonstrated that the discrete RSB solution of the SK model is not a consequence of the replica trick and the limit of the number of replicas to zero. Using real replicas we showed that the averaged free energy is an analytic function of the number of replicas on the positive axis. The thermodynamically formed ultrametric hierarchical structure with K levels of the order parameters in the SK model was shown to emerge due to thermodynamic inhomogeneity of the replica-symmetric solutions with less than K hierarchies. Thermodynamic homogeneity of the averaged free energy with respect to scalings (replications) of the phase volume is imposed at each hierarchical level. When not fulfilled, the free energy depends on the geometric scaling factor that is then chosen to minimize the inhomogeneity. It appears that in the SK model this minimization leads to maximization of the free energy. The number of hierarchical levels needed in this construction is fixed by the global homogeneity condition, Eq. (16a).

ACKNOWLEDGMENTS

The work on this problem was supported in part by Grant No. IAA1010307 of the Grant Agency of the Academy of Sciences of the Czech Republic and the ESF Programme SPHINX. The author thanks Lenka Zdeborová for fruitful discussions.

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