Incompleteness of the Thouless, Anderson, and Palmer mean-field description of the spin-glass phase

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(Received 20 December 2005; published 16 August 2006)

We analyze the low-temperature behavior of mean-field equations of Thouless, Anderson, and Palmer (TAP). We demonstrate that degeneracy in free energy makes the low-temperature TAP states unstable. Different solutions of the TAP equations, independent in the TAP approach, become coupled if an infinitesimal interaction between them is introduced. By means of real spin replicas we derive a self-averaging free energy free of unstable states with local magnetizations and homogeneous overlap susceptibilities between different spin replicas as order parameters. We thereby extend the TAP approach to a consistent description of the spin-glass phase for all configurations of spin exchange with (marginally) stable and thermodynamically homogeneous free energy.

DOI: 10.1103/PhysRevB.74.054207 PACS number(s): 64.60.Cn, 75.50.Lk

I. INTRODUCTION

The Parisi replica-symmetry breaking (RSB) scheme[1] was proved to be an exact solution of the Sherrington-Kirkpatrick (SK) model of spin glasses.[2] The analytic form of the mean-field theory of Ising spin glasses is hence known. What has not yet been unambiguously identified is the physical origin of the order parameters from the RSB solution of the replica trick. The replica trick is used to allow averaging of free energy over random configurations of spin couplings. Thermal and disorder-induced fluctuations are summed in the replica trick simultaneously via a single averaging of an n-times replicated partition function. One is hence unable to determine whether the former or the latter fluctuations give rise to the order parameters from the Parisi solution. To find the physical origin of the order parameters of the RSB solution one must separate the thermal and the disorder-induced fluctuations.

The direct thermodynamic approach summing separately the thermal fluctuations for fixed typical configurations of spin couplings J_{ij} in the SK model was pioneered by Thouless, Anderson, and Palmer.[3] The standard TAP theory of the SK model contains only local magnetizations m_i as order parameters. The averaging of the TAP free energy over random configurations within linear-response theory and with the fluctuation-dissipation theorem leads to the (replica-symmetric) SK solution unstable in the low-temperature phase.[4] That is, no Parisi RSB parameters emerge directly in the TAP theory.

The assumptions made for the averaging over randomness in the TAP theory are essentially equivalent to uniqueness of the equilibrium state for each relevant configuration of spin couplings. It appeared rather soon, however, that the TAP equations display a multitude of solutions in the spin-glass phase[5] resulting in a complex free-energy landscape of quasiequilibrium states.[6] The existence of multiple solutions of the TAP equations would not pose a problem if different states were distinguishable by symmetry-breaking fields introduced in free energy. The solutions of the TAP equations in the spin-glass phase are highly degenerate in free energy and cannot be singled out by external fields. Even worse is the fact that for a large number of configurations of spin couplings there are no stable states, local minima of the TAP free energy.[5,7] One hence cannot define a unique macroscopic thermodynamically stable state for these configurations. The existence of an exponentially large number of solutions of the mean-field equations has become a hallmark of spin-glass models. A new branch of research on complexity of solutions in the mean-field theory of spin glasses emerged.[8–11]

The nonexistence of thermodynamically stable macroscopic states for majority of configurations of spin couplings hinders the existence of the thermodynamic limit in the TAP approach. To circumvent this problem De Dominicis and Young suggested that the equilibrium state in the TAP approach be defined as a weighted sum over different TAP solutions.[12] That is, one assumes that the partition function can be represented as

$$\mathrm{Tr}_S \exp(-\beta H\{S\}) = \sum_{\alpha}^{\mathcal{N}} \exp(-\beta F_{\mathrm{TAP}}\{m_i^\alpha\}), \tag{1}$$

where $\mathcal{N}$ is the number of TAP solutions labeled by superscript α. Assumption (1) means that the phase space of the SK model is effectively disconnected. It consists of pockets of spin configurations corresponding to different TAP solutions separated by impenetrable infinite energy barriers.

Albeit assumption (1) defines a relation between individual TAP solutions and the macroscopic thermodynamic state, it does not introduce the RSB order parameters. They emerge in the De Dominicis and Young completion of the TAP theory when the replica trick for averaging over random configurations of spin couplings is used. Without averaging over randomness we are able neither to verify Eq. (1) nor to trace down the genesis of the RSB order parameters beyond the replica trick.

Averaging over randomness should not generally be the eventual tool for introducing the RSB order parameters. Guerra and Toninelli recently proved that the free energy of the SK model is self-averaging.[13] Should the TAP approach be exact, one must trace down the Parisi order parameters within the TAP approach without resorting to averaging over randomness. A question then arises whether the TAP construction indeed provides a complete description of the thermodynamics of the SK model.

We know that to derive the TAP theory we must assume uniqueness of the thermodynamic equilibrium state described by a set of local magnetizations. This, however, is the case only if a convergence condition for the linked-cluster expansion

$$1 \geqslant \frac{\beta^2 J^2}{N} \sum_i (1 - m_i^2)^2 \tag{2}$$

holds.[14] Equality in the above condition determines the de Almeida-Thouless (AT) line separating the high-temperature from the spin-glass phase along which the spin-glass susceptibility diverges.[15] Condition (2) is broken below the AT line for a macroscopic portion of spin-coupling configurations and the TAP free energy does not have an adequate (rigorous) justification there. We must continue analytically the TAP thermodynamic potentials from the high-temperature phase, where Eq. (2) is obeyed, to the low-temperature one, where the latter condition may be broken. Such a procedure is not uniquely defined, unless we have appropriate symmetry-breaking fields at our disposal. Presently, it is assumed that there are only local magnetic fields, Legendre conjugates to the local magnetizations, as symmetry-breaking forces. The TAP free energy in the spin-glass phase consequently has the same form as in the high-temperature phase, i.e., it is described by the same order parameters, local magnetizations m_i.

Recently Plefka suggested that the TAP equations in situations with unstable states where Eq. (2) is broken should be stabilized by introducing a new "order parameter," a correction to the local magnetic susceptibility beyond the fluctuation-dissipation theorem.[16] Plefka's extended solution, however, does not allow for a diagrammatic representation, the order parameter for the deviation from the fluctuation-dissipation theorem cannot be derived from free energy, and hence a physical meaning cannot be given to the calculations containing the TAP solutions breaking condition (2). Although the unstable states seem to become marginally stable in the thermodynamic limit,[17] the number of states breaking condition (2) linearly increases with the number of lattice sites and diverges in the thermodynamic limit.[5,7] Unstable states from large but finite volumes hence remain statistically relevant also in the thermodynamic limit, since the negative values of the rhs of Eq. (2) vanish with power $N^{-2/3}$.[10,17] We hence cannot disregard or inappropriately treat the finite-volume unstable states without further considerations. We can deduce that the number of TAP configurations with unstable states is macroscopically relevant in the thermodynamic limit also indirectly when averaging the TAP free energy over spin couplings J_{ij}. Using linear response and the fluctuation-dissipation theorem, equivalent to self-averaging property of free energy of ergodic systems, we fail to produce a thermodynamically stable equilibrium state in the spin-glass phase. Since we know that the exact free energy of the SK model is self-averaging, the TAP construction breaks down in the spin-glass phase. To attain a self-averaging configurationally-dependent free energy we must extend consistently the TAP free energy also to configurations with unstable states, i.e., beyond the validity of inequality (2).

The aim of this paper is to demonstrate that the TAP free energy becomes unstable whenever stability condition (2) is broken and the TAP equations do not have a single solution independent of the initial conditions. By using spin replicas for portions of the phase space belonging to different TAP solutions we show that linear response theory is broken when an infinitesimal interaction between different spin replicas (solutions of the TAP equations) is introduced. This breakdown generates a set of new homogeneous order parameters, overlap susceptibilities between different replicas. They lift degeneracy in the TAP free energy and break independence of different solutions of the TAP equations. We derive a generalization of the TAP free energy for one configuration of spin couplings containing site-dependent local magnetizations M_i and homogeneous local overlap susceptibilities χ^{ab} as order parameters. The latter are directly related to the RSB order parameters of the Parisi solution. In the paramagnetic phase $\chi^{ab}=0$ and we recover the TAP free energy. In the low-temperature phase, for configurations of spin couplings for which condition (2) is broken, the overlap susceptibilities become nonzero and we observe macroscopic deviations from the TAP free energy. Different solutions of the TAP equations are hence not separated by infinite energy barriers. Mutual thermodynamically induced interaction between solutions of the TAP equations mediated by the overlap susceptibilities interconnects parts of the phase space separated in the TAP theory. The phase space becomes simply connected and stable macroscopic thermodynamic states exist for each configuration of spin couplings independently of whether condition (2) is fulfilled or not. The interaction between different TAP states also leads to the existence of a single equilibrium state with a well-defined thermodynamic limit generated from a self-averaging free energy functional.

The paper is organized as follows. In Sec. II we recall the basic ingredients of the TAP theory with restrictions on its applicability. We use real replicas and the demand of thermodynamic homogeneity to extend (analytically continue) the TAP approach to situations with unstable TAP states in Sec. III. In Sec. IV we reduce the general theory to one hierarchical level and present the modified TAP equations, study their stability and finally demonstrate explicitly near the critical point that the TAP construction indeed becomes unstable in the spin-glass phase. In the last section we summarize our findings and discuss their consequences.

II. TAP MEAN-FIELD THEORY AND STABILITY OF ITS EQUILIBRIUM STATES

We first recall the basic concepts of the TAP theory for the SK model so that we understand the restrictions under which the TAP theory is applicable. In the diagrammatic representation the TAP free energy was derived as a sum of tree and single-loop (cavity-field) contributions with specific restrictions of the SK model on spin couplings J_{ij}, namely $\sum_j J_{ij}^{2n+1}=0$ and $\sum_j J_{ij}^2 = J^2$.[18] Due to the fluctuation-dissipation theorem the local susceptibility containing the loop contributions is a function of the local magnetization and the TAP free energy for the SK model is a functional of only local magnetizations m_i. It is convenient to represent the TAP free energy in the following form:

$$F_{\mathrm{TAP}} = \sum_i \left(m_i \eta_i^0 - \frac{1}{\beta} \ln 2 \cosh[\beta(h + \eta_i^0)] \right) - \frac{1}{2} \sum_{ij} \left(J_{ij} m_i m_j + \frac{1}{2} \beta J_{ij}^2 (1 - m_i^2)(1 - m_j^2) \right), \quad (3)$$

where we introduced apart from local magnetizations m_i also internal inhomogeneous magnetic field η_i^0. The sets of parameters m_i and η_i^0 are Legendre conjugate variables and are treated variationally in free energy (3). That is, they have to determine an extremal value of this free-energy functional. The corresponding stationarity (TAP) equations for these parameters read

$$m_i = \tanh[\beta(h + \eta_i^0)], \quad (4a)$$

$$\eta_i^0 = \sum_j J_{ij} m_j - m_i \sum_j \beta J_{ij}^2 (1 - m_j^2). \quad (4b)$$

These equations can now be solved numerically for finite numbers of lattice sites and given configurations of spin couplings. But not all solutions of equations (4) are physical ones. Only locally stable solutions for which the nonlocal susceptibility does not contain negative eigenvalues are meaningful. The inverse of the susceptibility is defined as a second derivative of free energy (3),

$$(\chi^{-1})_{ij} = \frac{\partial^2 \beta F_{\mathrm{TAP}}}{\partial m_i \partial m_j} + \sum_l \left(\frac{\partial^2 \beta F_{\mathrm{TAP}}}{\partial m_i \partial \eta_l^0} \frac{\partial \eta_l^0}{\partial m_j} + \frac{\partial^2 \beta F_{\mathrm{TAP}}}{\partial m_j \partial \eta_l^0} \frac{\partial \eta_l^0}{\partial m_i} \right) + \sum_{kl} \frac{\partial^2 \beta F_{\mathrm{TAP}}}{\partial \eta_k^0 \partial \eta_l^0} \frac{\partial \eta_k^0}{\partial m_i} \frac{\partial \eta_l^0}{\partial m_j} = -\beta J_{ij} + \delta_{ij} \left(\frac{1}{1 - m_i^2} + \sum_l \beta^2 J_{il}^2 (1 - m_l^2) \right). \quad (5)$$

That is, only local minima of the TAP free energy (3) as a functional of local magnetizations m_i, when the internal magnetic fields are resolved, are physically acceptable.

Non-negativity of the eigenvalues of the linear susceptibility is not the only stability criterion. There is a stronger condition on consistency of the TAP theory. It is connected with the existence of a nondegenerate equilibrium state, an assumption used in the derivation of the TAP free energy. This condition is expressed as positivity of the spin-glass susceptibility χ_{SG}. It is easy to find by summing the leading-order (N^{-1}) diagrammatic contributions[5] that the spin-glass susceptibility has in the SK model the following representation:

$$\chi_{\mathrm{SG}} \equiv \frac{1}{N} \sum_{ij} \chi_{ij}^2 = \frac{1}{N} \sum_i \frac{\chi_{ii}^2}{1 - \sum_j \beta^2 J_{ij}^2 \chi_{jj}^2}. \quad (6a)$$

This representation of the spin-glass susceptibility was derived diagrammatically but it is valid quite generally as long as the right-hand side (rhs) of Eq. (6a) remains non-negative, that is if

$$1 \geqslant \sum_j \beta^2 J_{ij}^2 \chi_{jj}^2. \quad (6b)$$

We show in Appendix A that representation (6a) can be derived also nonperturbatively using a theorem of Pastur and continuity of the resolvent for the inverse nonlocal susceptibility.

Realizing that the local susceptibility in the TAP theory reads

$$\chi_{ii} = 1 - m_i^2 \quad (6c)$$

we find that the stability condition from Eq. (2) equals the condition on positivity of the spin-glass susceptibility, Eq. (6b). Positivity of the spin-glass susceptibility is a feature that each consistent solution must possess. If it is broken, then the phase space of the order parameters is incomplete and some relevant fluctuations have not been taken into account appropriately. Note that in general positivity of the spin-glass susceptibility does not coincide with positivity of the eigenvalues of the nonlocal susceptibility. Only squares of the eigenvalues of the latter contribute to the former. The spin-glass susceptibility may become negative even if the linear susceptibility is positive, that is for a local minimum of the TAP free energy.

The TAP theory was derived assuming that the resulting free energy leads to a single (nondegenerate) stable thermodynamic state. That is, the TAP equations (4) lead to a single physical solution that can be separated from nonphysical ones by finite energy gaps. We know, however, that this is not the case in the spin-glass phase. Hence the TAP free energy is internally consistent only in the high-temperature phase, where it leads to a single stable equilibrium state. One must be more careful when extending the TAP approach to the low-temperature phase. There we cannot separate the physical solutions of the TAP equations from the nonphysical ones breaking stability condition (2). We must modify the TAP approach to situations with many quasiequilibrium and unstable states degenerate in free energy.

III. THERMODYNAMIC HOMOGENEITY AND MULTIPLE TAP STATES

The existence of many solutions of the TAP equations degenerate in free energy hinders the existence of a stable macroscopic equilibrium state and does not allow to perform the thermodynamic limit. In a degenerate case we cannot fix a single solution when enlarging the volume of the system and large fluctuation do not extinguish in the thermodynamic limit. Different unstable solutions of the TAP equations degenerate in free energy can be distinguished only by initial conditions, being the only input to Eqs. (4). This means that the TAP free energy is effectively not thermodynamically homogeneous, since it does not depend only on spatial densities of extensive variables. One way to handle a multitude of quasiequilibrium states in the TAP approach is to assume infinite barriers between different TAP states (independence of different solutions of the TAP equations) and use Eq. (1).

We can, however, avoid assumption (1) in that we do not *a priori* exclude interaction between different TAP states. Since different solutions of the TAP equations belong in the beginning to independent separate parts of the phase space, we can introduce for each TAP solution its own replica of the spin variables and sum up thermal fluctuations for each solution separately. This is actually the concept of real replicas that has been used by the author to derive the RSB solution from the demand of thermodynamic homogeneity of the averaged free energy.[19] In the TAP approach without averaging over randomness we can give a transparent physical interpretation to real spin replicas.

Let us assume that we have ν different TAP solutions (distinguished by their history). Since different solutions are initially thermodynamically independent we introduce independent spin replica for each TAP solution and replicate ν-times the original phase space. The partition function on this replicated phase space can be represented as $(\mathrm{Tr}\, e^{-\beta H})^{\nu} = \mathrm{Tr}_{\nu} \exp(\beta \Sigma_{a=1}^{\nu} H^{\alpha}) = \mathrm{Tr}_{\nu} \exp[\beta \Sigma_{a=1}^{\nu}(\Sigma_{i,j} J_{ij} S_i^a S_j^a + \Sigma_i S_i^a)]$, where 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. The free energy of a ν-times replicated system is just ν-times the free energy of the nonreplicated one, if it is thermodynamically homogeneous. We now break independence of individual spin replicas and add a small (infinitesimal) homogeneous perturbation breaking replica independence $\Delta H(\mu) = \Sigma_i \Sigma_{a<b} \mu^{ab} S_i^a S_i^b$. We could also break replica independence inhomogeneously by a site-dependent symmetry-breaking field μ_{ii}^{ab}. Since the stability condition for the TAP theory, Eq. (2), is global, we are effectively able to break replica dependence only globally as we demonstrate in the next section.

It is not the field μ^{ab} connecting different replicas that is of physical interest. We are interested in the linear response of the system to this perturbation. We derived[18] that after switching off the field μ^{ab} the ν-times replicated TAP free energy reads

$$\begin{aligned} F_{\nu} = \frac{1}{\nu}\sum_{a=1}^{\nu}\Bigg[& \sum_i M_i^a\left(\eta_i^a + \beta J^2 \sum_{b=1}^{a-1} \chi^{ab} M_i^b\right) \\ & - \frac{1}{4}\sum_{i,j} \beta J_{ij}^2 [1-(M_i^a)^2][1-(M_j^a)^2] \\ & - \frac{1}{2}\sum_{i,j} J_{ij} M_i^a M_j^a + \frac{\beta J^2 N}{2}\sum_{b=1}^{a-1} (\chi^{ab})^2 \Bigg] \\ & - \frac{1}{\beta\nu}\sum_i \ln \mathrm{Tr} \exp\left(\beta^2 J^2 \sum_{a<b}^{\nu} \chi^{ab} S_i^a S_i^b + \beta \sum_{a=1}^{\nu} (h+\eta_i^a) S_i^a\right). \end{aligned} \tag{7}$$

In this expression local magnetizations M_i^a and local internal magnetic fields η_i^a are configurationally dependent Legendre conjugate variational variables determined from stationarity equations analogously to the TAP equations (4). Apart from these parameters we introduced χ^{ab}, $a \neq b$, averaged overlap local susceptibilities representing a linear response to the replica-mixing field μ^{ab}. They are global (translationally invariant) variational variables, Legendre conjugates to the symmetry breaking fields μ^{ab}. It is straightforward to verify that at the saddle point we have $\chi^{ab} = N^{-1}\Sigma_i[\langle S_i^a S_i^b\rangle_T - \langle S_i^a\rangle_T \langle S_i^b\rangle_T]$, where $\langle\cdots\rangle_T$ stands for thermal averaging.

Free energy F_{ν} from Eq. (7) becomes independent of the replication index ν and reduces to the TAP free energy if $\chi^{ab}=0$. This is just the case when the convergence criterion for the TAP theory, Eq. (2), holds. A difference between the original TAP free energy and that from Eq. (7) emerges only in regions with unstable states in the TAP equations. Free energy (7) can hence be viewed upon as a general form of the TAP-like free energy for one configuration of spin couplings. Different replica indices correspond to different solutions of mean-field equations. Unlike the TAP approach the different states in free energy (7) are allowed to interact via the overlap susceptibility χ^{ab}.

If free energy F_{ν} is thermodynamically homogeneous it should not depend on the replication parameter ν. We already know that this is not the case, at least for the averaged TAP free energy, when stability condition (2) is broken.[19] If thermodynamic homogeneity is broken we must use the new order parameters so as to restore this fundamental property. Only thermally homogeneous systems possess nondegenerate stable equilibrium states extremizing a free-energy functional and can be extended uniquely to infinite volumes. In our construction, it is the matrix of overlap susceptibilities that should restore thermodynamic homogeneity in the TAP approach.

We now impose the condition of thermodynamic homogeneity on free energy (7) in that we demand the existence of a unique thermodynamic state. That is, all spin replicas must be equivalent and must lead to the same order parameters. This property can be quantified as follows:

$$M_i^a \equiv \langle S_i^a\rangle_T = M_i, \tag{8a}$$

$$\chi^{ab} = \chi^{ba}, \tag{8b}$$

$$\{\chi^{a1},\ldots,\chi^{a\nu}\} = \{\chi^{b1},\ldots,\chi^{b\nu}\}. \tag{8c}$$

Equation (8a) says that at the level of local magnetizations different spin replicas are indistinguishable. That is, the internal local magnetic fields are replica independent, $\eta_i^a = \eta_i$. Conditions (8b) and (8c) restrict the matrix of overlap susceptibilities to be symmetric with rows (columns) being only permutations of each other. We remind that $\chi^{aa}=0$. The matrix χ^{ab} contains then only $\nu-1$ independent parameters. that can be cast into groups of identical values. If we set $\nu_K > \nu_{K-1} > \cdots \nu_! > 1$ we may choose $\nu_1 - 1$-times a value χ_1, $(\nu_2 - \nu_1)$-times an overlap χ_2, and so on up to $(\nu_K - \nu_{K-1})$-times an overlap χ_K.

As the last step we must determine the structure of the matrix χ^{ab} with the above restrictions that would lead to an analytic free-energy functional of variables $\nu_1,\ldots,\nu_K$ and $\chi_1,\ldots,\chi_K$. The easiest way to determine the most general available structure of χ^{ab} is to use a hierarchical construction. It starts with $K=1$ and increases the number of different values of the overlap susceptibilities only if the solution with K different values becomes unstable. In the case $K=1$ the matrix of the overlap susceptibilities is uniquely determined by a multiplicity ν_1 of the only value χ_1. We examine this particular case in detail in the next section. If the theory with $K=1$ is unstable, we build up a theory with $K=2$ values of the overlap susceptibility, χ_1 and χ_2. We assume that not only the individual replicas are equivalent but also blocks of replicas describing the solution with $K=1$ are equivalent. That is, the diagonal elements in the solution with $K=1$ are replaced by matrices $\nu_1\times\nu_1$ with zero on the diagonal and χ_1 on the off-diagonal positions. The remaining off-diagonal elements in the solution with $K=2$ are filled with the value χ_2. In this way we go on to higher hierarchies. We end up with an ultrametric structure of the Parisi RSB solution. It is of essential importance that the ultrametric structure allows for an analytic representation of the hierarchical free energy with K different values of the overlap susceptibility. In fact, the ultrametric arrangement of the overlap susceptibilities χ^{ab} seems to be the most general structure in which the free energy is an analytic function of parameters χ_l, ν_l for $l=1,\ldots,K$.

Inserting the ultrametric structure with K hierarchies of χ^{ab} in Eq. (7) and after K-times applied the Hubbard-Stratonovich transformation linearizing the spin variables in the exponent of $\exp(\beta^2J^2\Sigma_{a<b}\chi^{ab}S_i^aS_i^b)$ we obtain an analytic representation of the K-level hierarchical generalization of the TAP free energy

$$F_K(\chi_1,\nu_1,\ldots,\chi_K,\nu_K) = -\frac{1}{4}\sum_{i,j}\beta J_{ij}^2(1-M_i^2)(1-M_j^2) - \frac{1}{2}\sum_{i,j}J_{ij}M_iM_j + \sum_i M_i\left(\eta_i + \frac{1}{2}\beta J^2 M_i\sum_{l=1}^{K}(\nu_l-\nu_{l-1})\chi_l\right) + \frac{\beta J^2 N}{4}\sum_{l=1}^{K}(\nu_l-\nu_{l-1})\chi_l^2 + \frac{\beta J^2 N}{2}\chi_1 - \frac{1}{\beta\nu_K}\sum_i \ln\left[\int_{-\infty}^{\infty}\mathcal{D}\lambda_K\left(\cdots\int_{-\infty}^{\infty}\mathcal{D}\lambda_1\left\{2\cosh\left[\beta\left(h+\eta_i+\sum_{l=1}^{K}\lambda_l\sqrt{\chi_l-\chi_{l+1}}\right)\right]\right\}^{\nu_1}\cdots\right)^{\nu_K/\nu_{K-1}}\right]. \quad (9)$$

We abbreviated $\mathcal{D}\lambda_l \equiv d\lambda_l e^{-\lambda_l^2/2}/\sqrt{2\pi}$ and used $\nu_0=1$, $\chi_{K+1}=0$. Notice that in our derivation $\nu_1<\nu_2<\cdots<\nu_K=\nu$ and $\chi_1>\chi_2>\cdots>\chi_K\geqslant 0$. Free energy (9) should be an extremum with respect to matrix χ^{ab} so that a thermodynamically homogeneous free energy is produced. Thermodynamic homogeneity is achieved in free energy (9) if it does not depend on ν_K. This is equivalent to vanishing of χ_K. Since the trivial solution $\chi_l=0$ always satisfies the stationarity equations for any $l=1,\ldots,K$, free energy (9) with K hierarchies is thermodynamically homogeneous if $\chi_K=0$ is the only physical solution of the respective stationarity equation. Nonexistence of a nontrivial solution for χ_K determines the number of hierarchical levels needed to achieve a globally stable solution.

Both sets of parameters χ_l and ν_l must be treated variationally and their physical values must be determined from respective stationarity equations. The equilibrium multiplicity factors ν_l^{eq}, determined from $\partial F_K/\partial\nu_l=0$, no longer need be integers, form an increasing sequence, and they even can be smaller than one. As discussed in Ref. 19 the stationarity equations for ν_l have two solutions, $\nu_l^{\mathrm{eq}}\geqslant 1$ and $\nu_l^{\mathrm{eq}}\leqslant 1$. The latter case is actually the physical one, since it minimizes thermodynamic inhomogeneity, if it occurs. The value $\nu_l<1$ determines then a portion of the phase space (relative number of lattice sites) of one TAP solution influenced by the existence of other TAP solutions. With a homogeneous, site-independent overlap susceptibility all spins in each solution are equivalent. The exponent ν_l then says that νN spins on average are influenced by other TAP solutions.[19]

Free energy (9) is the most general analytic continuation of the TAP free energy to the low-temperature phase. If condition (2) is obeyed for $\chi_l=0$, $l=1,\ldots,K$ and $F_K(\chi_1,\nu_1,\ldots,\chi_K,\nu_K)=F_{\mathrm{TAP}}$. Free energy F_K is self-averaging and it is numerically identical with the RSB free energy with K hierarchical levels as derived in Ref. 19. In the extension of the TAP theory, Eq. (9), the RSB order parameters are induced by thermal fluctuations and serve as mediators of interaction between different TAP solutions.

IV. ONE-LEVEL HIERARCHICAL TAP THEORY

Representation (9) of a configurationally dependent free energy is rather complicated. It is a futile activity to try to solve the corresponding stationarity equations for a chosen configuration of spin couplings in full generality before exploring suitable simplifications. Moreover, it is not necessary to reconstruct the complete spatial distributions of site-dependent local magnetizations when we are interested in thermodynamic quantities determined by lattice sums. Since free energy (9) is self-averaging, in most situations we can replace the sums over the lattice sites by averages over the distribution of random spin couplings. Thereby we perform this averaging within linear response theory and with the fluctuation-dissipation theorem. That is, we use the same averaging rules to Eq. (9) as used on F_{TAP} in deriving the SK solution. This direct way of averaging of F_K leads to the Parisi solution with K hierarchical levels.[18,19]

To demonstrate explicitly that free energy (9) is a nontrivial extension of the TAP free energy in the low-temperature phase also for fixed configurations of spin couplings we resort our analysis of this free energy to the solution with $K=1$, that is, to the one-level hierarchical solution.

A. Stationarity equations

It is straightforward to reduce the general expression for the hierarchical free energy F_K to the case $K=1$ with $\chi_1=\chi$ and $\nu_1=\nu$. We obtain

$$F_1(\chi,\nu) = -\frac{1}{4}\sum_{i,j}\beta J_{ij}^2(1-M_i^2)(1-M_j^2) - \frac{1}{2}\sum_{i,j}J_{ij}M_iM_j + \frac{\beta J^2 N}{4}\chi[(\nu-1)\chi+2] + \sum_i M_i\left(\eta_i + \frac{1}{2}\beta J^2(\nu-1)\chi M_i\right) - \frac{1}{\beta\nu}\sum_i \ln\int \mathcal{D}\lambda_i\{2\cosh[\beta(h+\lambda_i J\sqrt{\chi}+\eta_i)]\}^\nu. \tag{10}$$

Free energy $F_1(\chi,\nu)$ is represented in closed form and is analytic in all its variables M_i, η_i, χ, and ν. It reduces to the TAP expression if $\chi=0$, which is the case when Eq (2) is fulfilled by the local magnetizations M_i.

The stationarity equation for the site-dependent local magnetization follows from $\partial F_1/\partial\eta_i=0$ from which we obtain

$$M_i = \langle\rho^{(\nu)}(h+\eta_i;\lambda,\chi)\tanh[\beta(h+\eta_i+\lambda J\sqrt{\chi})]\rangle_\lambda \equiv \langle\rho_i^{(\nu)}t_i\rangle_\lambda, \tag{11a}$$

where

$$\rho_i^\nu \equiv \rho^{(\nu)}(h+\eta_i;\lambda,\chi) = \frac{\cosh^\nu[\beta(h+\eta_i+\lambda J\sqrt{\chi})]}{\langle\cosh^\nu[\beta(h+\eta_i+\lambda J\sqrt{\chi})]\rangle_\lambda} \tag{11b}$$

is a density matrix. We denoted $\langle X(\lambda)\rangle_\lambda = \int\mathcal{D}\lambda X(\lambda)$.

The internal local magnetic field η_i is determined from $\partial F_1/\partial M_i=0$ which results in

$$\eta_i = \sum_j J_{ij}M_j - M_i\left(\beta J^2(\nu-1)\chi + \sum_j \beta J_{ij}^2(1-M_j^2)\right). \tag{11c}$$

In addition to the site-dependent order parameters we must determine the physical (stationary) values of the homogeneous parameters χ and ν. From the equation $\partial F_1/\partial\chi=0$ we obtain

$$\chi = \frac{1}{N}\sum_i(\langle\rho_i^{(\nu)}t_i^2\rangle_\lambda - \langle\rho_i^{(\nu)}t_i\rangle_\lambda^2). \tag{12a}$$

The multiplicity parameter ν is derived from $\partial F_1(\chi,\nu)/\partial\nu=0$ leading to an explicit equation

$$\nu = \frac{4}{\beta^2J^2}\frac{N^{-1}\sum_i\{\langle\ln\cosh[\beta(h+\eta_i+\lambda J\sqrt{\chi})]\rangle_\lambda - \ln\langle\cosh^\nu[\beta(h+\eta_i+\lambda J\sqrt{\chi})]\rangle_\lambda^{1/\nu}\}}{\chi(2Q+\chi)}, \tag{12b}$$

where we denoted $Q\equiv N^{-1}\Sigma_i M_i^2$.

Global equations (12) complete local stationarity equations (11). Free energy, Eq. (10), together with stationarity equations (11) and (12) define an analytic theory in the entire space of the input parameters. They reduce to the TAP theory in the high-temperature phase but generally differ from it in the spin-glass phase. The spin-glass phase is characterized apart from local magnetizations also by two global parameters χ and ν. The principal difference between free energy F_1 and F_{TAP} is in the λ integral. This integration stands for thermal equilibration of the replicated spins, that is, for summations of spin configurations in the phase space determining other TAP solutions. Alternatively we can understand the λ integration as a thermally weighted averaging of the initial conditions for the TAP equations. Due to the dependence of TAP states on the initial conditions an additive homogeneous internal magnetic field $\lambda J\sqrt{\chi}$ emerges. If the interaction between different TAP solutions (initial and final configurations of local magnetizations) vanishes, $\chi=0$, free energy F_1 reduces to F_{TAP}.

There are also other situations, when $F_1=F_{\mathrm{TAP}}$. If $\nu=1$, functional F_1 is independent of χ and we recover the TAP free energy. The TAP free energy is recovered also in the limits $\nu\to\infty$ and $\nu\to 0$. In the former case the λ integration reduces to a saddle point at which $\nu\chi=\Gamma^2<\infty$. We explicitly obtain the limiting $\nu\to\infty$ value of free energy

$$\bar{F}_1(\Gamma,\bar{\lambda}_i) = -\frac{1}{4}\sum_{i,j}\beta J_{ij}^2(1-M_i^2)(1-M_j^2) - \frac{1}{2}\sum_{i,j}J_{ij}M_iM_j + \sum_i M_i\left(\eta_i+\frac{1}{2}\beta J^2\Gamma^2 M_i\right) + \frac{1}{\beta}\sum_i\left(\frac{\bar{\lambda}_i^2}{2} - \ln\{2\cosh[\beta(h+\eta_i+J\Gamma\lambda_i)]\}\right) \tag{13}$$

being now a functional of M_i, $\bar{\lambda}_i$, and Γ. At the saddle point

$\bar{\lambda}_i=\beta J\Gamma M_i$ and we find that $\partial\bar{F}_1/\partial\Gamma\equiv 0$, that is, free energy F_1 in the limit $\nu=\infty$ does not depend on Γ and we recover the TAP free energy.

In the limit $\nu\to 0$ the annealed randomness in the fluctuating field λ reduces to a quenched one and the one-level hierarchical free energy reduces to

$$F_1(\chi,0)=\frac{\beta J^2 N}{4}\chi(2-\chi)-\frac{1}{4}\sum_{i,j}\beta J_{ij}^2(1-M_i^2)(1-M_j^2)-\frac{1}{2}\sum_{i,j}J_{ij}M_iM_j+\sum_i M_i\left(\eta_i-\frac{1}{2}\beta J^2\chi M_i\right)-\frac{1}{\beta}\sum_i\int\mathcal{D}\lambda_i\ln\{2\cosh[\beta(h+\eta_i+\lambda_i J\sqrt{\chi})]\}. \tag{14}$$

In this representation we can absorb the fluctuating field λ_i into the internal magnetic field η_i and add the Gaussian λ integration to the summation over the lattice sites. After the substitution $\xi_i=\eta_i+\lambda_i J\sqrt{\chi}$ we find $\chi=1-Q$, where again we denoted $Q=N^{-1}\Sigma_i M_i^2$, and recover the TAP free energy.

It is clear from the above analysis that Eq. (12b) has always two solutions, one for $\nu<1$ and the second for $\nu>1$. In the former case it is a maximum of free energy and in the latter one it is a minimum. We show in the next section that the solution for $\nu>1$ is an unstable extremum of free energy (10) and hence the only physically acceptable, stabilizing extension of the TAP free energy is that with $\nu<1$. Free energy (10) offers a physical interpretation of the order parameters χ and ν. The last term on the left-hand side (lhs) of Eq. (10) is the genuine interacting part of the free energy. It is a local free energy of Ising spins in a random magnetic field $\lambda_i J\sqrt{\chi}$ due to spin configurations of the replicated spins (other TAP solutions). The λ integral stands for thermal averaging of the replicated spins and the exponent $\nu<1$ expresses a weight with which the replicated spins affect the local partition function. That is, effectively just νN spins are influenced by configurations of the replicated spins.

B. Stability conditions

Saddle-point equations (11) and (12) should lead to an extremum of free energy $F_1(\chi,\nu)$. The free energy for fixed homogeneous parameters χ and ν as a functional of only local magnetizations M_i, when Eq. (11c) for the local magnetic field is used, should be a minimum. Only then the nonlocal susceptibility is positive semidefinite. The nonlocal susceptibility in the one-level hierarchical TAP theory is defined analogously as in the standard TAP theory and reads

$$(\chi^{-1})_{ij}=-\beta J_{ij}+\delta_{ij}\left(\beta^2J^2[1-Q-(1-\nu)\chi]+\frac{1}{\chi_{ii}}\right). \tag{15}$$

The local inhomogeneous susceptibility in this case is

$$\chi_{ii}=1-M_i^2-(1-\nu)(\langle\rho_i^{(\nu)}t_i^2\rangle_\lambda-\langle\rho_i^{(\nu)}t_i\rangle_\lambda^2). \tag{16}$$

The fundamental consistency condition (positivity of the spin-glass susceptibility) is Eq. (6b) with the local susceptibility χ_{ii} from Eq. (16) and reads

$$1\geqslant\frac{\beta^2J^2}{N}\sum_i[1-(1-\nu)\langle\rho_i^{(\nu)}t_i^2\rangle_\lambda-\nu\langle\rho_i^{(\nu)}t_i\rangle_\lambda^2]^2. \tag{17}$$

If this condition is fulfilled free energy $F_1(\chi,\nu)$ from Eq. (10) is a physically acceptable and consistent solution for local magnetizations M_i, homogeneous overlap susceptibility χ and multiplicity factors ν. It is evident from Eq. (17) that if a TAP solution breaks condition (2), that is Eq. (17) for $\nu=1$, and we increase ν to higher values we worsen the instability of the TAP solution. To improve upon the incurred instability of the TAP solution we must evidently decrease the multiplicity factor ν to values lower than 1. That is, we must maximize free energy with respect to the matrix of overlap susceptibilities.

If Eq. (17) does not hold we are unable to find a stable equilibrium state that would not depend on initial conditions and would be separable from other macroscopic states by a finite gap in free energy. The degeneracy of the TAP free energy hence has not been lifted in free energy (10) completely. To improve upon this deficiency we must go to a theory with a higher number of hierarchies $K>1$. It is evident that the two-level free energy $F_2(\chi_1,\nu_1,\chi_2,\nu_2)$ reduces to $F_1(\chi,\nu)$ if either $\chi_2=0$ or $\chi_1=\chi_2$. It is straightforward to demonstrate that breakdown of condition (17) leads to an instability of equality $\chi_2=0$ and the second overlap susceptibility χ_2 starts to peel off from its zero value.

In the generalized TAP theory with local magnetizations M_i, internal magnetic fields η_i and homogeneous overlap susceptibilities $\chi_1,\nu_1,\ldots,\chi_K,\nu_K$ as order parameters, minimization of the TAP free energy with respect to local parameters does no longer play an essential role for stability of macroscopic states. This condition is replaced in the hierarchical extension of the TAP theory by a more important condition, an extremum with respect to the homogeneous order parameters, overlap susceptibilities χ_l with their multiplicities ν_l for $l=1,2,\ldots,K$. Extremum of the hierarchical free energy with respect to homogeneous parameters leads to an extremum in thermodynamic inhomogeneity of free energy. Since only $\nu_l<1$ lead to minimization of thermodynamic inhomogeneity, we must maximize free energy to achieve the least inhomogeneous state. Free energy F_1 may hence also become unstable when the one-level solution does not maximize free energy and solutions with a higher number of hierarchical levels (different values for the overlap susceptibilities) produce a higher free energy. This happens if equation $\chi_2=\chi_1$ becomes unstable and a new value of $\chi_2<\chi_1$ emerges. This happens if the following stability condition is broken[19]

$$1\geqslant\frac{\beta^2J^2}{N}\sum_i\langle\rho_i^{(\nu)}(1-t_i^2)^2\rangle_\lambda. \tag{18}$$

Unlike Eq. (17) condition (18) gets stabilized with increasing ν. In the TAP theory with $\chi=0$ both conditions coincide.

It is necessary that both conditions, Eqs. (17) and (18), are satisfied for the equilibrium values of all order parameters so that free energy (10) leads to stable thermodynamic states for almost all configurations of spin couplings. It depends on the equilibrium value of the parameter ν which of these two conditions is (more) broken and hence responsible for the eventual instability of the one-level TAP free energy F_1. It is Eq. (18) that makes the solution for $\nu \to 0$ unstable, TAP free energy from Eq. (14). It is Eq. (17) that leads to instability of solutions with $\nu \to 1$, TAP free energy (3). Note that in the averaged theory the relevant instability condition of the extended TAP theory corresponds to the stability of the one-step RSB scheme.

C. Asymptotic solution near the critical point

Stationarity equations (11) and (12) in full generality are difficult to solve for a fixed configuration of spin couplings. One can, however, investigate the behavior of the order parameters close to the spin-glass transition. In particular, one can explicitly confirm that the TAP solutions become unstable below the spin-glass transition whenever condition (2) is broken. We prove in this section that if Eq. (2) is broken the overlap susceptibility χ becomes positive and the multiplicity factor $\nu \in (0,1)$ deviates from its equilibrium value from the high-temperature phase.

The small parameter in the low-temperature phase is the overlap susceptibility. We hence expand all necessary quantities from stationarity equations (11) into powers of χ. We will need the two leading nontrivial orders. The asymptotic form of the local magnetization at the AT line reads

$$M_i \doteq \mu_i - \beta^2 J^2 (1-\nu)\mu_i (1-\mu_i^2)\chi + \beta^4 J^4 (1-\nu)\mu_i (1-\mu_i^2)[2-\nu-(3-2\nu)\mu_i^2]\chi^2, \tag{19}$$

where we denoted $\mu_i = \tanh[\beta(h+\eta_i)]$. In expansion (19) we assumed that the internal magnetic field is fixed, although its stationary value also depends on χ. This dependence will be evaluated at the end of our calculations.

The difference on the rhs of Eq. (12a) must be expanded into the first two orders in χ. We obtain with the above notation

$$\langle \rho_i^{\nu)} t_i^2 \rangle_\lambda - \langle \rho_i^{(\nu)} t_i \rangle_\lambda^2 \doteq \beta^2 J^2 (1-\mu_i^2)^2 \chi - \beta^4 J^4 (1-\mu_i^2)^2 [2-\nu-(8-5\nu)\mu_i^2]\chi^2. \tag{20}$$

We will need to expand the global parameter $Q = N^{-1}\Sigma_i M_i^2$ in Eq. (12b). Also this parameter must be expanded to the first two powers of χ. We obtain directly from Eq. (19),

$$Q \doteq \langle \mu_i^2 \rangle_{\text{av}} - 2\beta^2 J^2 (1-\nu)\langle \mu_i^2 (1-\mu_i^2)\rangle_{\text{av}}\chi + \beta^4 J^4 (1-\nu) \times \langle \mu_i^2 (1-\mu_i^2)[5-3\nu-(7-5\nu)\mu_i^2]\rangle_{\text{av}}\chi^2, \tag{21}$$

where we abbreviated $\langle X_i \rangle_{\text{av}} = N^{-1}\Sigma_i X_i$. This notation, originating in self-averaging property of local variables, we also use in the following formulas.

Next we denote

$$\varphi = \frac{4}{\beta^2 N}\sum_i \{\langle \ln \cosh[\beta(h+\eta_i+\lambda J\sqrt{\chi})]\rangle_\lambda - \ln\langle \cos h^\nu[\beta(h+\eta_i+\lambda J\sqrt{\chi})]\rangle_\lambda^{1/\nu}\}.$$

We expand this function to $O(\chi^3)$ and use it together with Eq. (21) for the evaluation of the expansion of both sides of Eq. (12b). Using the program MATHEMATICA we end up with

$$\Delta = \nu\chi(2Q+\chi) - \varphi \doteq \nu\chi^2\Big\{1-\beta^2 J^2 \langle (1-\mu_i^2)^2\rangle_{\text{av}} + \tfrac{2}{3}\beta^4 J^4 \chi \langle (1-\mu_i^2)^2 [3-2\nu-(11-8\nu)\mu_i^2]\rangle_{\text{av}}\Big\}. \tag{22}$$

Before we proceed with solving the asymptotic forms of equations (12a) and (12b) we must determine the χ dependence of the equilibrium value of the internal magnetic field η_i. It is sufficient for our purposes to expand this field only to linear power and we replace $\eta_i \to \eta_i^0 + \chi\dot{\eta}_i$. The local magnetization changes accordingly,

$$\mu_i \doteq m_i + (1-m_i^2)\chi\beta\dot{\eta}_i, \tag{23}$$

where we denoted $m_i = \tanh[\beta(h+\eta_i^0)]$ the TAP local magnetization with the fluctuating internal magnetic field η_i^0 determined by the TAP equation (4b). We derive an equation for $\beta\dot{\eta}_i$ from Eq. (11c). We have

$$\beta\dot{\eta}_i = \beta^2 J^2 [(1-\nu)+\dot{Q}]M_i + \sum_j [\beta J_{ij} - \delta_{ij}\beta^2 J^2 (1-Q)]\dot{M}_j. \tag{24a}$$

Further on, we obtain from Eq. (19) for $\dot{M}_i = dM_i/d\chi$ an asymptotic relation

$$\dot{M}_i \doteq (1-m_i^2)[\beta\dot{\eta}_i - \beta^2 J^2 (1-\nu)m_i]. \tag{24b}$$

The equation for $\dot{Q}$ follows directly from expansion (21).

Combing the above equations and using the definition for the TAP susceptibility we come to a solution

$$\beta\dot{\eta}_i \doteq \beta^2 J^2 (1-\nu)\left(m_i - 2\beta^2 J^2 \frac{\langle m_i^2 (1-m_i^2)\rangle_{\text{av}}}{(1-m_i^2)} \sum_j \chi_{ij}^{TAP} m_j\right). \tag{24c}$$

To reach a representation in closed form we must evaluate sums with the linear susceptibility of type $N^{-1}\Sigma_{ij}\chi_{ij}^{\text{TAP}} f(m_i) g(m_j)$. We derive an explicit formula for such sums in Appendix B.

With explicit expressions for the sums with the nonlocal susceptibility we have at hand all necessary ingredients to resolve the asymptotic form of equations for the global order parameters near the critical point. We first use Eq. (B11) to evaluate

$$\begin{aligned}\langle (1-\mu_i^2)^2\rangle_{\text{av}} &\doteq \langle (1-m_i^2)^2\rangle_{\text{av}} - 4\langle (1-m_i^2)^2 m_i \beta\dot{\eta}_i\rangle_{\text{av}}\chi \\ &= \langle (1-m_i^2)^2\rangle_{\text{av}} \\ &\quad + 4\beta^2 J^2 (1-\nu)\langle m_i^4 (1-m_i^2)\rangle_{\text{av}}\chi \\ &\quad - 8\beta^4 J^4 \langle m_i^2 (1-m_i^2)\rangle_{\text{av}}\langle m_i^2 (1-m_i^2)^2\rangle_{\text{av}}\chi.\end{aligned} \tag{25}$$

With this result the asymptotic form of the equation for the overlap susceptibility reads

$$\beta^2 J^2 \langle (1-m_i^2)^2 \rangle_{\rm av} - 1 \doteq \beta^4 J^4 \chi \{ \langle (1-m_i^2)[2-\nu-2(5-3\nu)m_i^2 + (4-\nu)m_i^4] \rangle_{\rm av} + 8\beta^2 J^2 (1-\nu) \langle m_i^2 (1-m_i^2) \rangle_{\rm av} \langle m_i^2 (1-m_i^2)^2 \rangle_{\rm av} \} \quad (26)$$

while the equation for the multiplicity factor ν can be rewritten to

$$\beta^2 J^2 \langle (1-m_i^2)^2 \rangle_{\rm av} - 1 \doteq \tfrac{2}{3} \beta^4 J^4 \chi \{ \langle (1-m_i^2)[3-2\nu - 2(7-5\nu)m_i^2 + (5-2\nu)m_i^4] \rangle_{\rm av} + 12\beta^2 J^2 (1-\nu) \langle m_i^2 (1-m_i^2) \rangle_{\rm av} \langle m_i^2 (1-m_i^2)^2 \rangle_{\rm av} \}. \quad (27)$$

Both equations (26) and (27) are in fact defining equations for the overlap susceptibility χ. The left-hand sides of both equations are identical and become positive in the low-temperature phase when condition (2) is broken. Since the solutions from both equations must lead to the same unique value of χ we must equal the right-hand sides of these equations. As a result we obtain an equation for the value of the parameter ν along the AT line of critical points. Its solution reads

$$\nu \doteq \frac{2\langle m_i^2 (1-m_i^2)^2 \rangle_{\rm av}}{\langle (1-m_i^2)^3 \rangle_{\rm av}}. \quad (28)$$

Parameter ν obtained from Eq. (28) is the limiting value of the low-temperature solution at the AT line. It is positive at finite magnetic field. This causes no problem, since we know that the high-temperature solution obeying the consistency condition (2) is independent of ν (thermodynamically homogeneous). To determine the deviation of ν from its value at the AT line in the spin-glass phase we must go to higher orders of the expansion in χ.

With the above solution for the multiplicity factor we can use either Eq. (26) or Eq. (27) to determine the overlap susceptibility χ. The solution for this parameter is physical only if the rhs of Eqs. (26) and (27) is positive. We can conclude already from Eq. (28) that this cannot be the case down to zero temperature along the AT line. The geometric parameter ν must be smaller than one. We have a critical value ν_c of this parameter at which the rhs of Eqs. (26) and (27) vanish, namely

$$\nu_c = 2\frac{\langle (1-m_i^2)(1-3m_i^2) \rangle_{\rm av} \langle (1-m_i^2)(1-3m_i^2+2m_i^4) \rangle_{\rm av}}{\langle (1-m_i^2)(1-4m_i^2) \rangle_{\rm av}^2 - \langle m_i^2 (1-m_i^2) \rangle \langle (1-m_i^2)(1-2m_i^2) \rangle_{\rm av} + \langle m_i^4 (1-m_i^2) \rangle \langle (1-m_i^2)(1-9m_i^2) \rangle_{\rm av}}. \quad (29)$$

Using the solution for ν from Eq. (28) on the lhs of Eq. (29) we obtain an equation for a critical value of the magnetic field (temperature) above (below) which the above asymptotic solution breaks down and we must go to higher-order terms in the expansion in the overlap susceptibility. We hence experience a crossover in the behavior of the homogeneous order parameters along the instability (AT) line if we go to high magnetic fields. While in low magnetic fields the overlap susceptibility is determined from a linear equation (26), we have a quadratic equation determining the leading asymptotic term near the AT line in high magnetic fields. The instability of the TAP equation in high magnetic fields is a rather complex task and will be presented in a separate presentation.

V. SUMMARY AND CONCLUSIONS

We analyzed the low-temperature thermodynamics of mean-field models of spin glasses. In particular, we concentrated on the behavior of thermodynamic potentials for individual configurations of spin couplings. For this purpose Thouless, Anderson, and Palmer proposed a construction of a configurationally dependent free energy of the Sherrington-Kirkpatrick model. The derivation of the TAP free energy is, however, valid only if a convergence or stability condition (2) is obeyed. Typical configurations of spin couplings in the spin-glass phase either do not allow for solutions of the TAP equations satisfying this condition or produce a multitude of solutions degenerate in free energy macroscopically many of which break Eq. (2). This situation naturally evokes a number of questions about the TAP construction: (1) Is it complete? (2) Does it produce stable equilibrium states? (3) Does the thermodynamic limit exist? Finally, we know that the exact solution of the SK model is the Parisi RSB scheme. The order parameters introduced by the replica trick are not manifested in the TAP thermodynamic potentials. Hence, we should answer another question: (4) At what stage do the RSB order parameters emerge?

Presently, it is predominantly assumed that the TAP theory is complete as it is and contains all necessary order parameters from which we can construct the exact solution. It does not produce a single equilibrium state, but rather exponentially many locally stable and unstable states separated by infinite energy barriers and (almost) degenerate in free energy. Hence a weighted sum (1) of local free-energy minima is to be taken into account to construct a global equilibrium state with which we can construct the thermodynamic limit. The only information missing in the TAP thermodynamic potentials is the complexity, i.e., the number of available TAP states, local minima of the TAP free energy. There is, however, no trace of the RSB order parameters in the TAP construction and they are introduced only in course of averaging over the quenched randomness in spin couplings.

In this paper we proposed alternative answers to the above urgent questions about the TAP construction and its relation to the RSB order parameters. We explicitly demonstrated that the TAP free energy for situations with broken stability condition (2) is unstable. The TAP approach becomes incomplete and must be enriched by new order parameters. The necessity for the enhancement of the TAP construction emerges due to the need to lift degeneracy in the TAP free energy that cannot separate stable from unstable states. Unlike the existing approaches we do not need to assume impenetrable energy barriers between different TAP states. We allow for energy flows between these states if it is thermodynamically convenient and if it leads to stabilization of equilibrium states. The energy flow between them is mediated and controlled by new homogeneous order parameters, overlap susceptibilities. These additional order parameters are determined thermodynamically from stationarity equations so that to achieve a thermodynamically homogeneous free energy with (marginally) stable equilibrium states. The overlap susceptibilities introduced in the proposed extension of the TAP construction of a configurationally dependent free energy are directly related to the Parisi RSB order parameters. They coincide after averaging over spin couplings. Since the configurationally dependent free energy with overlap susceptibilities is self-averaging, averaging over randomness is performed within linear response theory and with the fluctuation-dissipation theorem as in the case of the SK solution.

We demonstrated in this paper that the TAP construction is incomplete in the low-temperature phase, the TAP states are unstable and decay into a composite state described by inhomogeneous local magnetizations and homogeneous overlap susceptibilities. The extended free energy from which the physical values of the order parameters are determined is self-averaging with a well-defined equilibrium state and thermodynamic limit. The RSB order parameters, the overlap susceptibilities, emerge due to thermal fluctuations as mediators of interaction between different TAP states. Averaging over randomness is harmless and does not change the structure of the phase space of the order parameters.

When compared with the existing treatments of the thermodynamic behavior of spin-glass models we can conclude that the hierarchical TAP free energy (9) reduces to the TAP one for equilibrium states described by local magnetizations satisfying condition (2). The proposed extension of the TAP construction may then seem redundant, since only TAP solutions being local minima satisfying Eq. (2) are physically relevant. It is, however, not the case. The proper analytic continuation of the TAP approach to unstable states guarantees a consistent description of all states without a tedious way of the separation of locally stable and unstable solutions of the TAP equations. Moreover, the interaction between the TAP solutions introduced by the overlap susceptibilities changes the structure of the underlying phase space and the value of free energy. The hierarchical TAP theory does not require solving numerically the TAP equations for typical configurations of spin couplings in finite volumes or to calculate the complexity of the TAP theory. To determine thermodynamic properties of the SK model we can directly average the configurationally dependent free energy in the thermodynamic limit, which is a significant simplification.

ACKNOWLEDGMENTS

Research on this problem was carried out within a project AVOZ10100520 of the Academy of Sciences of the Czech Republic and was supported in part by Grant No. IAA1010307 of the Grant Agency of the Academy of Sciences of the Czech Republic.

APPENDIX A: SPIN-GLASS SUSCEPTIBILITY AND THE RESOLVENT

The averaged local susceptibility χ and the spin-glass susceptibility χ_{SG} can be derived from the resolvent constructed from the inverse nonlocal susceptibility. The inverse of the nonlocal susceptibility is a second derivative of free energy and can generally be represented as

$$(\chi^{-1})_{ij} = -\beta J_{ij} + \delta_{ij}\left(\frac{1}{\chi_{ii}} + \sum_j \beta^2 J_{ij}^2 \chi_{jj}\right). \qquad \text{(A1)}$$

The resolvent for a complex energy z (scaled by β in the same way as the inverse susceptibility) is defined

$$G(z) = \frac{1}{N}\mathrm{Tr}(z\hat{1} - \hat{\chi}^{-1})^{-1}. \qquad \text{(A2)}$$

The averaged local susceptibility and the spin-glass susceptibility can be derived from the resolvent as

$$\chi = \frac{1}{N}\sum_i \chi_{ii} = -G(0), \qquad \text{(A3a)}$$

$$\chi_{SG} = \frac{1}{N}\sum_{ij} \chi_{ij}^2 = -\left.\frac{dG(z)}{dz}\right|_{z=0}. \qquad \text{(A3b)}$$

In the Sherrington-Kirkpatrick model we have $\sum_j \beta^2 J_{ij}^2 \chi_{jj} = \beta^2 J^2 \chi = -\beta^2 J^2 G(0)$. We now use a theorem of Pastur[20] for the resolvent of matrices with off-diagonal elements being Gaussian random variables with variance J^2/N. When applied to the inverse susceptibility we obtain for $\Delta G(z) = G(z) - G(0)$,

$$\Delta G(z) = -\frac{1}{N}\sum_i \frac{\chi_{ii}^2[z - \beta^2 J^2 \Delta G(z)]}{1 - \chi_{ii}[z - \beta^2 J^2 \Delta G(z)]}. \qquad \text{(A4)}$$

Using the definition of the spin-glass susceptibility, Eq. (A3b) we obtain

$$\chi_{SG} = \frac{\dfrac{1}{N}\sum_i \dfrac{\chi_{ii}^2}{[1 + \beta^2 J^2 \Delta G(0)\chi_{ii}]^2}}{1 - \dfrac{\beta^2 J^2}{N}\sum_i \dfrac{\chi_{ii}^2}{[1 + \beta^2 J^2 \Delta G(0)\chi_{ii}]^2}}. \qquad \text{(A5)}$$

Assuming continuity of the resolvent at origin $z=0$ we have $\Delta G(0)=0$ and we end up with representation (6a).

Note that the resolvent representation (A4) does not exclude a nontrivial solution for $\Delta G(0)$. Setting $z=0$ in Eq. (A4) we obtain an equation

$$\Delta G(0) = \beta^2 J^2 \Delta G(0) \frac{1}{N} \sum_i \frac{\chi_{ii}^2}{1+\beta^2 J^2 \Delta G(0)\chi_{ii}} \tag{A6}$$

allowing for a nontrivial solution if the stability condition (2) is broken. This nontrivial solution was used by Plefka in Refs. 16 and 17 in his extension of the TAP theory. If we choose the nontrivial solution for $\Delta G(0)$ dictated by analyticity of the resolvent in the complex plane, the spin-glass susceptibility is no longer represented by Eq. (6a) but rather by Eq. (A5) and remains positive in the spin-glass phase. The new parameter $\Delta G(0) > 0$ cannot, however, be derived from a free energy and does not possess a diagrammatic representation. It is not a proper symmetry-breaking order parameter of microscopic origin. Moreover, with this parameter we break continuity of the resolvent and

$$\lim_{z\to 0} G(z) \neq G(0) = -\frac{1}{N}\sum_i \chi_{ii}. \tag{A7}$$

The last equality is the definition of the averaged local susceptibility, Eq. (A3a). The discontinuity makes a physical interpretation and explanation of the order parameter $\Delta G(0)$ difficult. We can only observe that positivity of $\Delta G(0)$ formally expresses a deviation from the fluctuation-dissipation theorem. There is no evidence or indication that the TAP solutions really lead to a discontinuous resolvent and $\Delta G(0) > 0$ in the spin-glass phase. An alternative way how to reach thermodynamic consistency and positivity of the spin-glass susceptibility within a microscopic construction provided by the hierarchical free energy with a fluctuation-dissipation theorem in the extended phase space with real spin replicas is offered in this paper.

APPENDIX B: SUMS WITH THE NONLOCAL MEAN-FIELD SUSCEPTIBILITY

The mean-field approximation is a single-site theory in that it effectively decouples distinct lattice sites. The decoupling of distinct lattice sites leads to a simplification of sums with nonlocal functions. These sums can be converted in the mean-field theory to uncorrelated lattice sums with site-local functions. Correlation between different sites enters mean-field expressions only via homogeneous global parameters being again uncorrelated sums over lattice sites.

In the spin-glass mean-field theory we are interested in sums with the nonlocal susceptibility of the form

$$C[f,g] = \frac{1}{N}\sum_{ij} \chi_{ij} f(m_i) g(m_j). \tag{B1}$$

The only nonlocal term in the susceptibility is the spin exchange βJ_{ij}. It is the off-diagonal part of the susceptibility that makes the evaluation of sums from Eq. (B1) difficult. We hence use the following representation for the nonlocal susceptibility:

$$\begin{aligned}\chi_{ij} &= \chi_{ii}\Big(\delta_{ij} + \sum_k{}' \beta J_{ik}\chi_{kj}\Big) \\ &= \chi_{ii} + \chi_{ii}\Big(\beta J_{ij} + \sum_k \beta J_{ik}\chi_{kk}\beta J_{kj} \\ &\quad + \sum_{k\neq j}\sum_{l\neq i} \beta J_{ik}\chi_{kk}\beta J_{kl}\chi_{ll}\beta J_{lj} + \cdots\Big)\chi_{jj},\end{aligned} \tag{B2}$$

where the primed sum does not allow for repetition of site indices. It means that only self-avoiding random walks contribute to the inverse matrix in the formal solution to Eq. (B2).

Representation (B2) can easily be proved by a diagrammatic expansion when the definition of the TAP susceptibility (5) is used. We successively exclude repeating site indices in the multiple sums of the expansion for the inverse of the rhs of expression (5). The diagonal element of the susceptibility χ_{ii} was determined along this line, e.g., in Ref. 5.

Since the site indices in Eq. (B2) are decoupled we can use the following functional representation for the spin exchange of the SK model

$$\beta J_{ij} = \frac{\beta^2 J^2}{N}(\nabla_i m_j + m_i \nabla_j). \tag{B3}$$

We denoted $\nabla_i \equiv \chi_{ii}\partial/\partial m_i$. Representation (B3) is a consequence of the fact that just squares of the spin coupling J_{ij} contribute to the sum $C[f,g]$. The paired spin exchange to the given one J_{ij} connecting lattice sites i and j can be extracted from the endpoint functions of local magnetizations m_i and/or m_j. A more detailed proof of Eq. (B3) can be found in Ref. 18.

Using Eq. (B3) we can represent the off-diagonal susceptibility $\widetilde{\chi}_{ij} = \chi_{ij} - \chi_{ii}\delta_{ij}$ as

$$\widetilde{\chi}_{ij} = \frac{\beta^2 J^2}{N}(\nabla_i \chi_{ii} m_j \chi_{jj} + m_i \chi_{ii} \nabla_i \chi_{jj} + \nabla_i X_j + m_i \chi_{ii} Y_j), \tag{B4}$$

where we denoted global parameters $X_j = \Sigma_k m_k \widetilde{\chi}_{kj}$ and $Y_j = \Sigma_k \nabla_k \widetilde{\chi}_{kj}$. Note that the differential operator ∇_i acts to the right on functions of the local magnetization m_i only. The lattice sums in the definition of the global parameters X_j and Y_j should avoid the fixed index j. In the mean-field approximation we can neglect this restriction, since the difference is only of order $O(N^{-1})$.

It is straightforward to find from Eq. (B4) an equation for

$$\begin{aligned}X_i &= \beta^2 J^2(\langle \nabla_k m_k \chi_{kk}\rangle_{\rm av} m_i \chi_{ii} + \langle m_k^2 \chi_{kk}\rangle_{\rm av} \nabla_i \chi_{ii} \\ &\quad + \langle \nabla_k m_k \chi_{kk}\rangle_{\rm av} X_i + \langle m_k^2 \chi_{kk}\rangle_{\rm av} Y_i),\end{aligned} \tag{B5}$$

where we denoted as in the main text $\langle X_k\rangle_{\rm av} \equiv N^{-1}\Sigma_k X_k$. Analogously we find

$$\begin{aligned}Y_i &= \beta^2 J^2(\langle \nabla_k \nabla_k \chi_{kk}\rangle_{\rm av} m_i \chi_{ii} + \langle \nabla_k m_k \chi_{kk}\rangle_{\rm av} \nabla_i \chi_{ii} \\ &\quad + \langle \nabla_k \nabla_k \chi_{kk}\rangle_{\rm av} X_i + \langle \nabla_k m_k \chi_{kk}\rangle_{\rm av} Y_i).\end{aligned} \tag{B6}$$

To represent the solution for these parameters concisely we denote $l = \beta^2 J^2 \langle (1-m_i^2)^2\rangle_{\rm av}$ and $r = \beta^2 J^2 \langle m_i^2 (1-m_i^2)\rangle_{\rm av}$. Then

$$X_i = \frac{(1-l)(l-2r)m_i\chi_{ii} + r\nabla_i\chi_{ii}}{(1-l)^2 + 2r(2-l)} \tag{B7}$$

and

$$Y_i = (2l-r)\frac{-2m_i\chi_{ii} + (1-l)\nabla_i\chi_{ii}}{(1-l)^2 + 2r(2-l)}. \tag{B8}$$

Inserting Eqs, (B7) and (B8) in Eq. (B4) we obtain

$$\chi_{ij} = \chi_{ii}\delta_{ij} + \frac{\beta^2 J^2}{N[(1-l)^2 + 2r(2-l)]} \times[(1+2r-l)(\nabla_i\chi_{ii}m_j\chi_{jj} + m_i\chi_{ii}\nabla_j\chi_{jj}) - 2(l-2r)m_i\chi_{ii}m_j\chi_{jj} + r\nabla_i\chi_{ii}\nabla_j\chi_{jj}]. \tag{B9}$$

Equation (B9) holds only in the leading N^{-1} order. Hence the second term on the rhs contributes only to the off-diagonal part and to lattice sums with the nonlocal susceptibility.

This representation is still a rather complicated expression. Fortunately, we need to know for our purposes the nonlocal susceptibility only along the AT line for which $l=1$. In this case the nonlocal susceptibility reduces to

$$\chi_{ij} = \chi_{ii}\delta_{ij} + \frac{\beta^2 J^2}{2N}(2\nabla_i\chi_{ii}m_j\chi_{jj} + 2m_i\chi_{ii}\nabla_j\chi_{jj} + \nabla_i\chi_{ii}\nabla_j\chi_{jj}) - \frac{\langle(1-m_k^2)(1-3m_k^2)\rangle_{\text{av}}}{\langle m_k^2(1-m_k^2)\rangle_{\text{av}}\langle(1-m_k^2)^2\rangle_{\text{av}}} m_i\chi_{ii}m_j\chi_{jj}. \tag{B10}$$

Using this result for functions $f(m_i)=m_i(1-m_i^2)$ and $g(m_j)=m_j$ in Eq. (B1) we find an explicit representation for a sum with the nonlocal susceptibility at the AT line needed in Eq. (25),

$$\frac{1}{N}\sum_{ij}\chi_{ij}m_i(1-m_i^2)m_j = \frac{\beta^2 J^2}{2}\langle(1-m_k^2)^2\rangle_{\text{av}}\langle(1-m_k^2) \times(1-3m_k^2)\rangle_{\text{av}}. \tag{B11}$$

Notice that the nonlocal susceptibility (B9) diverges at the critical point of the SK model only at zero magnetic field where $r=0$.

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