Modified Thouless-Anderson-Palmer equations for the Sherrington-Kirkpatrick spin glass: Numerical solutions

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(Dated: December 3, 2021)

For large but finite systems the static properties of the infinite ranged Sherrington-Kirkpatrick model are numerically investigated in the entire the glass regime. The approach is based on the modified Thouless-Anderson-Palmer equations in combination with a phenomenological relaxational dynamics used as a numerical tool. For all temperatures and all bond configurations stable and meta stable states are found. Following a discussion of the finite size effects, the static properties of the state of lowest free energy are presented in the presence of a homogeneous magnetic field for all temperatures below the spin glass temperature. Moreover some characteristic features of the meta stable states are presented. These states exist in finite temperature intervals and disappear via local saddle node bifurcations. Numerical evidence is found that the excess free energy of the meta stable states remains finite in the thermodynamic limit. This implies a ‘multi-valley’ structure of the free energy on a sub-extensive scale.

PACS numbers: 75.10.Nr, 05.50.+q, 87.10.+e

I. INTRODUCTION

The Sherrington-Kirkpatrick (SK) model [1] for Ising spins with quenched random bonds is the simplest representative of a class of long-ranged models all describing successfully the interesting phenomena of spin glasses [2, 3]. In addition to this success in physical questions, the research on these models has been fruitful and stimulating in optimization problems, in the understanding of neural networks and in the field of learning machines [2, 3]. In addition to this success in physical questions, the research on these models has been fruitful and stimulating in optimization problems, in the understanding of neural networks and in the field of learning machines [2, 3].

Two complimentary but conceptually different approaches exist for the analysis of these models. The first approach is the replica method applied already by Sherrington and Kirkpatrick to their model in the original work. After breaking the replica symmetry it was Parisi [5] who first found a satisfactory solution of the SK model in the spin glass regime.

Within the replica theory and the related dynamical approaches [1], an averaging over the quenched variables is performed and therefore only the calculation of bond averaged quantities is possible. All problems that depend on a special, but arbitrary configuration of the random bonds cannot be solved within the framework of the replica theory. Such problems are the generic case in the nonphysical applications named above. In optimization problems, for instance, the main question is to find the optimal solution for a fixed configuration.

The complimentary approach of Thouless-Anderson-Palmer (TAP) [6] to investigate spin glass models does not perform the bond average and permits the treatment of problems depending on specific configurations. For other questions which are expected to be independent of the special configuration, such as all macroscopic physical quantities, self averaging happens. This is due to the fact that the random interaction matrices have well known asymptotic properties in the thermodynamic limit [8]. The situation is in principle similar to the central limit theorem in probability theory, where large numbers of random variables also permit the calculation of macroscopic quantities which hold for nearly every realization of the random variables. Thus the investigation of one or some representative systems is sufficient and the bond average is not needed.

The TAP equations have been well established for more than two decades and several alternative derivations are known [2, 3, 9]. Nevertheless the TAP approach is still a field of current interest. This is due to the importance of the approach to numerous interesting problems. Moreover it is suspected that not all aspects of this approach have yet been worked out. Very recently the author [10] has reanalyzed the stability of the TAP equations. He concluded that the reason for the breakdown at the spin glass instability is an inconsistency in the value of the local susceptibility and showed that unstable states cannot be described by the original TAP equations. Removing these inconsistencies by a self-consistent treatment, modified TAP equations below the instability have been presented [10].

One of the pressing questions is the characteristic features of the pure states of the SK model, which are the stable solutions of the TAP equations. It is obvious that these states are essential for a direct understanding of the SK model. Moreover the pure states are of importance for the interpretation of the more formal results of the replica theory [2].

Apart from the research [11], showing that the number of the pure states is very large at low temperatures, two approaches exist to investigate the characteristic features of the pure states. Both the work of Bray and Moore [12] and the work of Nemoto and Takayama [13] try to find explicitly numerical solutions of the TAP equations for...
large but finite systems. Only in rare cases (about 15% of the systems with different bond configurations) do these investigations yield solutions of the TAP equations which satisfy the validity condition. To treat the other cases Nemo and Takayama have developed an interesting but indirect method to obtain at least approximative solutions which are expected to converge to true solutions in the thermodynamic limit. The applied numerical method of [13] did not work well for a cooling of the sample and therefore results for this case have not been published.

In this work we will demonstrate that all the known difficulties to find numerically the pure states disappear if the modified TAP equations [10] are applied instead of the original ones. For all configurations of the bonds, stable solutions of these TAP equations will be found for finite systems employing a simple relaxational dynamics. There is no further need to apply the indirect method of [13] and our approach permits the sample to be cooled down, as is shown to be essential to find the low lying states. In addition to these general goals some characteristic features of pure states will be worked out leading to a better understanding of the SK spin glass.

In Section II the basics of the modified TAP equations, some essentials of the applied dynamics and the numerical procedure are presented. A main subject of section III is the investigation of finite size effects which are found to be of some importance. The numerical results of the state of lowest free energy for the relevant static quantities will be given for all temperatures below the critical spin glass temperature. Next we focus on the meta stable states and discuss some characteristic features. Finally, the concluding remarks can be found in section IV.

II. BASIC EQUATIONS AND METHOD

A. The modified TAP equations

The Hamiltonian of the SK model of a system of N Ising spins \( S_i = \pm 1 \) in the presence of local external fields \( h_i \) is described by

\[
H = -\frac{1}{2} \sum_{i \neq j} J_{ij} S_i S_j - \sum_i h_i S_i .
\]

The bonds \( J_{ij} \) are independent random variables with zero means and standard deviations \( N^{-1/2} \) (where the latter scaling fixes the spin glass temperature to \( T = 1 \)).

The modified TAP mean field equations [10] describe the statics of the system (1) in the thermodynamic limit. They are given by the set of equations for the local magnetizations, with \( m_i = \langle S_i \rangle_\beta \)

\[
m_i = \tanh \beta \{ h_i + \sum_j J_{ij} m_j - m_i \chi_l \}
\]

together with the local susceptibility

\[
\chi_l = \frac{1}{N} \sum_i \frac{\beta(1 - m_i^2)}{1 + \beta^2 (1 - m_i^2)/2} \tag{3}
\]

and with

\[
\Gamma = 0 \quad \text{for } x \geq 0
\]

\[
1 = \frac{1}{N} \sum_i \frac{\beta^2 (1 - m_i^2)^2}{1 + \beta^2 (1 - m_i^2)^2} \quad \text{for } x \leq 0 \tag{5}
\]

where

\[
x = 1 - \beta^2 (1 - 2q_2 + q_4)
\]

and

\[
q_\nu = N^{-1} \sum_i m_i^{\nu} \quad \nu = 2, 4 \tag{7}
\]

was introduced.

The condition \( x = 0 \) represents the central spin glass instability condition [2, 3, 14]. Above the instability the local susceptibility \( \chi_l \) reduces to the isothermal value \( \chi_l^{(\beta)} \)

\[
\chi_l^+ = \chi_l^{(\beta)} = \beta (1 - q_2) \quad \text{for } x \geq 0
\]

which is in complete agreement with the original TAP approach [3, 9, 10]. Essential differences, however, result below the instability as

\[
\Gamma^- > 0 , \quad \chi_l^- \neq \chi_l^{(\beta)} \quad \text{for } x < 0
\]

holds for the modified TAP equations. According to [10] the quantity \( \Gamma \) is proportional to the density of zero eigenvalues of the inverse susceptibility matrix. Thus all the states with \( x < 0 \) are unstable. As thermodynamics does not apply to unstable states, a conflict with the exact thermodynamic point of view the modified equations are equivalent to the original TAP equations as thermodynamics is a priori limited to stable states. Note, however, that unstable states are essential for discussions based on free energy landscapes or for the extension to dynamics of the present approach. For a further discussion of this point we refer to [10] and to the end of the next subsection.

For later use we give the well known expressions [3, 9, 10] for the energy

\[
U = -\frac{1}{2} \sum_{i \neq j} J_{ij} m_i m_j - \beta \frac{2}{2} N(1 - q_2)^2 - \sum_i h_i m_i \tag{10}
\]

and the entropy

\[
S = -\sum_i \left\{ \frac{1 + m_i}{2} \ln \frac{1 + m_i}{2} + \frac{1 - m_i}{2} \ln \frac{1 - m_i}{2} \right\}
\]

\[- N \beta^2 \frac{4}{4} N(1 - q_2)^2 \tag{11}
\]
from which the free energy

\[ F = U - TS \]  

(12)
can be calculated. Note that these expressions were obtained by thermodynamic approaches. Hence they are restricted to stable states.

B. Glauber dynamics

As in [3, 15], Glauber dynamics in mean field approximation will phenomenologically be added to the model. Measuring the time \( t \) in units of the relaxation time, the purely relaxational equations of motion are given by

\[ \dot{m}_i(t) = -m_i + \tanh \beta \{ h_i + \sum_j J_{ij} m_j - m_i \chi_l(t) \}. \]

(13)
The local susceptibility \( \chi_l(t) \) is related to the \( m_i(t) \) via eq.(4) and via eq.(3) or eq.(5) depending on the instantaneous value of \( x(t) \). The fixpoints of these equations of motion obviously coincide with the solutions of the modified TAP equations.

To analyze the dynamical stability of these fixpoints the equations of motion are linearized near a fixpoint \( m_i \). Setting

\[ \delta m_i(t) = m_i(t) - m_i \]

(14)
and neglecting as usual the \( N^{-1} \) order terms \( \propto \partial \chi_l / \partial m_i \), the linearized equations take in matrix notation the form

\[ \delta \dot{m} = -\chi_0 \chi^{-1} \delta m \]

(15)
where \( \chi_0 \) represents the static susceptibility matrix for noninteracting Ising spins

\[ (\chi_0)_{ij} = \beta (1 - m_i^2) \delta_{ij} \]

(16)
and where

\[ \chi^{-1} = \chi_0^{-1} + \chi_l \mathbf{1} - \mathbf{J} \]

(17)
is the inverse of the susceptibility matrix of the modified TAP approach [10]. For thermodynamic stable or marginal stable states \( \chi^{-1} \) is positive semi-definite.

According to eq.(15) the dynamical stability is governed the matrix \( \Lambda = \chi_0 \chi^{-1} \). Let \( l \) be an eigenvector of \( \Lambda \) satisfying the eigenvalue equation \( \Lambda l = \lambda l \). Multiplication with \( \chi_0^{-1} \) leads to \( \chi^{-1} l = \lambda \chi_0^{-1} l \) and to

\[ \lambda = \frac{l \cdot \chi^{-1} l}{l \cdot \chi_0^{-1} l}. \]

Immediately \( \lambda \geq 0 \) results from the definiteness of \( \chi_0 \) and of \( \chi^{-1} \) for stable (or meta stable) static states. Static stability therefore implies dynamical stability. By a similar argument, the statement can be proven in the opposite direction, leading to a one-to-one correspondence between the two types of stability.

The latter result implies that the stable solutions of the TAP equations can be found by integration of the equations of motions (13). The system relaxes to a stable fixpoint which is certainly located outside the regime \( x < 0 \). For transient times, however, the system can enter the regime \( x(t) < 0 \) and thus the flow of eqs.(13) is needed in both regions \( x(t) < 0 \) and \( x(t) > 0 \). These arguments demonstrate the relevance of the unstable states and consequently the need for the modified TAP equations for the present approach. It should be added that equations of motion of the above type but based on the original TAP equations usually lead to incorrect results in the spin glass region. For this case the system generally relaxes to paramagnetic solutions.

C. Systems of finite size

The modified TAP equations are exact in the thermodynamic limit but are approximative for systems of finite size. As numerical studies can only be performed for finite systems the two approximations yielding to eqs.(4) for finite \( N \) are recalled.

First of all eqs.(2) holds only to leading order in \( N^{-1} \) as sub-extensive contributions have been neglected (compare e.g. appendix of [10]). Further corrections to eq.(2) result from the application [10] of the Pastur theorem [16] which is again only exact in the thermodynamic limit. The explicit form of these two types of corrections are not known and seem to be hard to determine analytically. Hence the finite size effects resulting from the two approximations will be investigated empirically in the numerical section.

Due to the sub-extensive corrections the border of stability \( x = 0 \) is expected to be only approximative for finite systems. This implies that unstable solutions with \( x > 0 \) and stable solutions with \( x < 0 \) may exist for systems of finite size. Such stable solutions with \( x < 0 \) and \( \Gamma > 0 \) are indeed found in the following.

Finally it is pointed out that the results of subsection B are not restricted to the thermodynamic limit and hold for systems of all sizes. Thus the fixpoints obtained by integration of the eqs.(13) always correspond to stable solutions of the modified TAP equations.

D. Numerical procedure

The numerical investigations are performed for systems up to a size of \( N = 225 \) with binary distributions of the bonds \( J_{ij} = \pm N^{-1/2} \) using the standard routine ‘NIntegrate’ of Mathematica on workstations.

The integration of the equations of motion (13) in the regime \( x(t) > 0 \) is straightforward. In the region \( x(t) < 0 \), however, a special procedure is employed and \( (\beta T)^2 \) is treated as additional dynamical variable. The time derivative of eq.(14) yields the necessary additional
equation of motion and the initial value of $(\beta \Gamma)^2$ is determined from eqs.\((\ref{3})\) for $t = 0$ which finally guarantees that eq.\((\ref{3})\) is satisfied for all times.

During the dynamic evolution $x(t)$ generally changes sign, which implies a change of the numerical treatment. Therefore an alternative, approximative approach is partly applied. Instead of eq.\((\ref{3})\) the equation

$$1 = \frac{c}{N T^2} + \frac{1}{N} \sum_i \frac{\beta^2 (1 - m_i^2)^2}{1 + \Gamma^2 \beta^2 (1 - m_i^2)^2} \quad \quad (18)$$

is used, where $c$ is a small positive constant with typical values from $10^{-3}$ to $10^{-5}$. With the supplementary term $c/(NT^2)$ eq.\((\ref{15})\) has a solution $\Gamma > 0$ for all values of $x$. Due to the smallness of $c$ only small differences occur in comparison with the exact values of $\Gamma$, which are $\Gamma = 0$ for $x > 0$ or which, for the case $x < 0$, are determined by eq.\((\ref{3})\). Hence the set of eqs.\((\ref{13}), (\ref{3})\) and \((18)\) can be used for all values of $x(t)$ leading to an unified treatment of the cases $x < 0$ and $x > 0$. No significant differences are found for the results of these two methods.

In the numerical investigations of the next section the results are presented as functions of the temperature from $T = .01$ to $T = 1$. The temperature variation is performed both step-wise and continuously. Usually the step size is $\Delta T = .01$. For the case of continuous variations the temperature is linearly and slowly changed. Typically $10^5$ relaxation times are taken, to change the temperature from $T = 0.1$ to $T = 1$.

For runs at a fixed temperature with $N = 100$ and with $N = 225$, several minutes and a couple of hours are needed, respectively. It takes, however, several hours for $N = 100$ and several days for $N = 225$ when the temperature is continuously changed in the entire interval. At low temperature $T < .1$ the numerical integration is more time consuming than at higher temperatures.

### III. NUMERICAL RESULTS

#### A. Finite size effects

Let us first discuss two trivial finite size effects. The largest eigenvalue $J_{\text{max}}$ of the interaction matrix $J$ determines the spin glass temperature $T_{sg} = J_{\text{max}}/2$. For finite $N$ this eigenvalue $J_{\text{max}}$ differs from the $N \to \infty$ value $\frac{\beta}{2}$ of $2$. The deviations are of the order of $5\%$ and mainly arise near $T = 1$.

The second simple effect results at low temperatures. The binary distributions $J_{ij} = \pm N^{-1/2}$ imply a splitting of the energy levels of $\Delta E = 2N^{-1/2}$. Thus for temperatures $T \ll 2N^{-1/2}$ only the ground state properties enter into the calculation of thermodynamic quantities, which causes atypical effects for temperature below $T = .1$. These effects are not discussed in the following \cite{17}.

For an analysis of the convergence of the present approach with increasing $N$ we investigate systems of the size $N = 16, 25, 36, 49, 64, 81, 100, 121, 196$ and $225$. For each size with $N \leq 121$ one hundred different realizations of the bonds are investigated. For the systems with $N = 196$ and with $N = 225$ thirty bond configurations are examined in each case. The temperature is fixed at $T = .5$ and all calculations are performed in zero field. Starting with random initial values the system relaxes always to a fixpoint of the equation of motion that is different from the paramagnetic solution $m_i = 0$.

The fixpoint solutions are classified in two classes. In the majority class (containing about $85\%$ of all solutions), the value of $\Gamma$ is finite and the solutions are located in the region $x < 0$. The solutions of the minority class satisfy $x > 0$ and $\Gamma = 0$. Both classes are already known in literature \cite{12,13} and related to the cases where solutions of the original TAP equations are not found or are found \cite{18}.

The minority class corresponds to the case were the
TAP free energy has a local minimum. As shown in [12, 13], the obtained $x$ values of these solutions tend to zero for $N \to \infty$ and the minimum tends to a marginally stable saddle point. Our data are in complete agreement for most systems.

For $N = 225$ (sample I) which is representative for most systems. All solutions of the this class have a finite values for $\Gamma$ and satisfy $l \leq 0$, which is a significant dependence on the asymptotic behavior of both quantities.

We focus the discussion on the majority class. All solutions of this class have a finite values for $\Gamma$ and satisfy $x < 0$. Both results are caused by the finite size of the systems, as for $N \to \infty$ all solutions of the modified TAP equations with these properties are unstable. Thus it is expected that both $\Gamma$ and $x$ tend to zero when approaching the thermodynamic limit. Fig.3 and Fig.4, where the averaged $\Gamma^2$ and the averaged $x$ are plotted against $N^{-2/3}$, show indeed this expected behavior. The data are consistent - but not conclusively - with a $N^{-2/3}$ dependence for the asymptotic behavior of both quantities.

From the viewpoint of the modified TAP equations both classes are similar. The solutions of the minority class and of the majority class describe the approach to $x = 0$ from above and from below, respectively. As $x = 0$ represents the boundary of stability in the thermodynamic limit, this viewpoint clearly shows the asymptotic marginal stability of the TAP solutions in the glassy state.

Turning to temperature dependent effects we will present results for three specific systems. From the majority class we select sample I and sample II with sizes $N = 225$ and $N = 100$, respectively. Sample III with a size of $N = 100$ is chosen from the minority class.

With the aim of finding the states with lowest free energy we slowly cool down the systems to $T = 0.01$, starting at $T = 1$ with the paramagnetic solution as initial values. For sample I in zero field the numerical results for $x, \Gamma, \chi_l$ and $\chi_l^{(b)} = \beta (1 - q_2)$ are presented in Fig.4. The spin glass instability is approached from below for nearly all temperatures, where $x < 0$, $\Gamma > 0$ and $\chi_l \neq \chi_l^{(b)}$ hold. The results for sample III are different and are plotted in Fig.5. In this sample whether the instability is approached from above or from below is dependent on the temperature.

In Fig.4 and Fig.5 discontinuities of $\chi_l, \Gamma$ and $x$ arise which result from saddle node bifurcations and which are discussed in some detail in Sec. III.D. These jumps are expected to disappear in the thermodynamic limit. In this case we have $x \to 0$ and $\Gamma \to 0$ and thus $\chi_l(\to \chi_l^{(b)})$ will become a smooth curve. Quite remarkably the figures show that $\chi_l \to 0$ holds for $T \to 0$, which is a desired behavior found in other approaches [2, 3].

The procedure of slowly cooling down to get the states of lowest free energy can at best be justified by empirical arguments. Indeed, further states of the samples under investigation were found to have in general, but not always a higher free energy (compare Sec. III.C.).

To obtain some more evidence for this procedure, we apply our approach to systems with zero fields and with $N = 10, 11, \ldots 22$ and investigate for each $N$ one hundred sets of the bonds. In each case the state of lowest free energy at $T = 0$ is determined by slowly cooling down from $T = 1$ and compared with the exact result which can be calculated due to the smallness of the systems. We obtain agreement in 95% of all cases and in a further 4% of the cases the cooling method found one of the, in general degenerate, lowest exited states. A significant dependence on $N$ is not found. Provided that an extrapolation to large $N$ is possible, these results are quite remarkable, even from the viewpoint of optimization problems.
FIG. 5: Edwards Anderson order parameter of the state of lowest free energy: $q_2$ versus temperature $T$ in zero field (full line) and in external fields $h$ for sample I with $N = 225$ (dotted lines) and for sample II with $N = 100$ (dashed lines). At the temperatures where the lines for finite fields end the glassy regime is entered and $x$ becomes negative. The dots represent the results of the replica approach [20] for $h = 0$.

FIG. 6: Total magnetization of the state of lowest free energy: $m = N^{-1} \sum m_i$ versus temperature in external fields $h$ for sample I with $N = 225$ (full lines) and for sample II with $N = 100$ (dashed lines). The dashed dotted line shows the SK results ending at the AT temperature and the dots mark the temperatures where $x$ changes sign.

FIG. 7: Energy density of the state of lowest free energy: $u = U/N$ versus temperature $T$ in external fields $h$ for sample I with $N = 225$.

FIG. 8: Entropy density of the state of lowest free energy: $s = S/N$ versus temperature $T$ in external fields $h$ for sample I with $N = 225$. The dots represent the results of the replica approach [20] for $h = 0$.

could be improved by rescaling the temperature axis to identical spin glass temperatures.

In Fig. 5 the $T$ and $h$ dependence of the total homogeneous magnetization $m = N^{-1} \sum m_i$ is presented. This figure also shows the result of the replica theory [1] above the AT line [4] being exact in the thermodynamic limit. Again the finite size effects are relatively large. The general behavior, however, can clearly be identified.

The energy density $u = U/N$ and the entropy density $s = S/N$ are plotted in Fig. 7 and in Fig. 8, respectively. Only the results for sample I are given, as the differences to sample II are not resolved on the scale of these figures.

For the calculation of the plotted quantities eq. (10) and eq. (11) are used. This use implies again an approximation, as strictly these asymptotic equations hold only for $\Gamma = 0$. Note finally that the results of Fig. 8 are again in agreement to the results of [20] based on the replica approach.
approach.

C. Meta stable states

Let us estimate the expected number of solutions $N_s$ of the TAP equations for our system sizes. At $T = 0.2$, according to Bray and Moore [21], this number is approximately given by $N_s \approx \exp(0.05 N)$. In zero magnetic field for each solution a further solution can trivially be constructed by changing the sign of all $m_i$. Counting each pair as one independent solution the estimates for the number of independent solutions are 75 and 3850 for $N = 100$ and $N = 225$, respectively. Note that the basis for this estimate are the original and not the modified TAP equations and thus these numbers should be used with some care for the present work.

The investigations for finding meta stable sates are performed in zero external field at $T = 0.2$, starting each run with different random initial values of the $m_i$.

In 540 runs we have found 74 independent solutions of the modified TAP equations for sample II. In the first 100 runs nearly one half of them are obtained. Afterwards the rate for finding new solutions quickly decreases to about 8% and remains approximately constant for later runs. Thus certainly not all existing solutions of this sample are observed. The statistical results, presented in the following, are nearly independent of the solutions of later runs. This implies that the observed solutions are representative for all solutions of this sample. A further argument for the last statement results from the fact that the states with the 8 lowest free energies are found in the first 100 runs. This preference for the lower states is also found in the rate of recurrence of all runs, which indicates a large basin of attraction for these states.

For sample I with $N = 225$ we have calculated 868 different states in 1250 runs. For this sample the rate for finding new solutions decreases only to a value of about 50%. Nevertheless it is assumed that the solutions found are again representative for all solutions. In this context it should be added that about 8% of the meta stable states of both samples have a $x > 0$ and belong therefore to the minority class.

Fig 9 shows the normalized distribution $W(\Delta F)$ of the excess free energy $\Delta F = F - F^0\epsilon$ at $T = 0.2$ in zero field for sample I (full line) and for sample II (dashed line). The smooth line shows a Gaussian fit of the data of sample I.

Assuming that the findings can be generalized this is an interesting result for the 'multi-valley structure' of the free energy. It implies that all the possible excess free energies $\Delta F^\alpha$ remain finite in the thermodynamic limit. Note that this conclusion is in agreement with the result of [10] that the 'multi-valley' structure of the TAP free energy occurs on a sub-extensive scale.

Let us introduce the overlap $q^\alpha\alpha'$ between the solution $m_i^\alpha$ and the solution $m_i^\alpha'$ in the usual way

$$q^\alpha\alpha' = N^{-1} \sum_i m_i^\alpha m_i^\alpha'$$

and define the normalized, white-weighted overlap distribution

$$P_w(q) = \frac{2}{\hat{N}_s(N_s - 1)} \sum_{\alpha < \alpha'} \delta(q - q^\alpha\alpha').$$

where $\hat{N}_s$ denotes the total number of solutions. (Note that $P_w(q)$ is not the Parisi overlap distribution, as the Boltzmann weights are absent.)

The distribution $P_w(q)$ is symmetrical in $q$ and is plotted for $q > 0$ as histogram in Fig.10 for samples I and for sample II. Both distributions are similar and thus nearly independent of the system size $N$. The resulting asymptotic distribution seems to be a Gaussian distribution. Such a distribution would result if all the directions of the meta stable states in the $N$ dimensional space are not correlated.
FIG. 11: **Meta stable states:** Excess free energy $\Delta F$ of sample I versus temperature $T$ of the six lowest and four further meta stable states which can be reached by physical processes (compare text). The full and the dotted lines correspond to $x < 0$ and $x > 0$, respectively and the dashed arrows indicate the observed jumps when changing $T$. The insert shows the details of a hysteresis near a discontinuity.

Unfortunately the data for the meta stable states are not sufficient to answer the interesting question of whether the Parisi overlap distribution, a quantity averaged over all bonds $J_{ij}$, applies also to single systems. Both samples have just three states with non negligible Boltzmann weights and thus definitive conclusions are impossible.

The temperature dependence of the meta stable states is presented for (at $T = .2$) the lowest six and some higher states of sample I in Fig.11. The branches of the latter states can be reached by physical processes. These processes consist of a slow field cooling part which starts at $T = 1$ and which is followed by a sudden switching-off of the field at $T = .2$. For the values $h = 1.5, h = 1.0, h = .5$ and $h = 1$ the processes end at the points A,B,C and D of Fig.11 respectively.

All the meta stable states investigated vary smoothly in some temperature region which is limited by an upper limiting temperature. Above this temperature the states disappear via saddle node bifurcations. For some states an additional lower limiting temperature is found (compare insert of Fig.11). The system remains in a definite meta stable state for all slow changes of the temperature as long as the limiting temperatures are not reached. However approaching a limiting temperature by slow temperature changes, the system always bifurcates into a branch which has a lower free energy, implying hysteresis effects in some cases. Although such results are physically expected this behavior is numerically verified for all states plotted in Fig.11.

Note that in the whole temperature range most of the meta stable states have negligible Boltzmann weights. Actually only the three lowest states of sample I will give non negligible contributions to Boltzmann averaged quantities. Nevertheless the system will remain dynamically in a meta stable state of high free energy for all times provided it remains there initially and provided no drastic changes of the temperature or the magnetic field are performed.

According to Fig.11 the free energy levels sometimes cross with changes of the temperature. Even the state of lowest free energy can be involved, which implies that the state of lowest free energy and the first exited state change their roles at the crossing temperature. Thus in the notations of this work, to call the state slowly cooled from $T = 1$ the state of lowest free energy is not strictly correct. For brevity we will still use this term keeping, however, the limitations in mind.

### D. Saddle node bifurcations

In this subsection the discontinuities are analyzed which arise in the temperature dependence of states of lowest free energy and of the meta stable states.

For this purpose the eigenvalues $\lambda^{(m)} \leq \lambda^{(1)} \leq \lambda^{(2)} \ldots$ and the eigenvectors $u^{(m)}$ of the inverse susceptibility \[ \chi^{-1} u^{(m)} = \lambda^{(m)} u^{(m)} \quad m = 0,1 \ldots N - 1. \] are introduced for an arbitrary solution $m_i$ at the temperature $T$. Approaching a discontinuity the smallest eigenvalue $\lambda^{(0)}$ tends to zero and vanishes at a critical temperature $T_c$. In Fig.12 an example is presented where the temperature dependence of $\lambda^{(0)}$ is given by the numerical solutions of eq.(21).

For further discussions the staggered magnetizations $\Delta m^{(m)}$ are defined \[ \Delta m^{(m)} = \sum_i \{ m_i(T) - m_i(T_c) \} u_i^{(m)}(T_c) \quad m = 0,1 \ldots \] (22)

The numerical results for $\Delta m^{(0)}$ and $\Delta m^{(1)}$ are plotted in Fig.12 for a discontinuity. Within the numerical errors $\Delta m^{(0)} \sim (T_c - T)^3$ and $\Delta m^{(1)} \sim (T_c - T)$ hold where the latter result is representative for all $m \neq 0$.

These temperature variations can analytically be explained. For such an approach eq.(2) is rewritten as \[ h_i(T,m_k) = \frac{T}{2} \ln \frac{1 + m_i}{1 - m_i} - \sum_j J_{ij} m_j + m_i \chi \] (23)
and expanded at \( T_c \) to first order in \( \Delta T = T_c - T \) and to second order in \( \Delta m_i = m_i(T) - m_i(T_c) \) which yields

\[
A_i \Delta T = \sum_j \chi_{ij}^{-1} \Delta m_j + \sum_{jk} \frac{B_{ijk}}{2} \Delta m_j \Delta m_k \tag{24}
\]

with

\[
A_i = \partial_T h_i(T, m_k)|_{T_c} \text{ and } B_{ijk} = \partial_{mk} \chi_{ij}^{-1}(T, m_k)|_{T_c}. \tag{25}
\]

Multiplying eq. (24) from the left by the eigenvectors \( u^{(\alpha)}(T_c) \) the \( \Delta m^{(\alpha)} \) are calculated to

\[
\Delta m^{(\alpha)} = \pm \sqrt{2A^{(\alpha)}/B^{(\alpha)}} \Delta T + O(\Delta T^{3/2}) \tag{26}
\]

and to

\[
\Delta m^{(\alpha \neq 0)} = \frac{A^{(\alpha)}B^{(0)} - A^{(0)}B^{(\alpha)}}{B^{(\alpha)}/\chi^{(\alpha)}(T_c)} \Delta T + O(\Delta T^{3/2}) \tag{27}
\]

where

\[
A^{(\alpha)} = \sum_i u_i^{(\alpha)}(T_c) A_i \tag{28}
\]

and

\[
B^{(\alpha)} = \sum_{ijk} u_i^{(\alpha)}(T_c) B_{ijk} u_j^{(0)}(T_c) u_k^{(0)}(T_c). \tag{29}
\]

The analytic results (24) and (26) agree with temperature dependence found numerically and plotted in Fig. 12.

Moreover these results exhibit all the typical features of a saddle-node bifurcation. The two branches exist only for \( \Delta T > 0 \) or for \( \Delta T < 0 \) depending on the signs of \( A^{(0)} \) and of \( B^{(0)} \). Provided the branches exist one of them is stable and the other is unstable.

The staggered magnetizations \( \Delta m^{(0)} \) govern the behaviors of the states near the critical temperatures. Thus the \( \Delta m^{(0)} \) are the order parameters of the local saddle node bifurcations.

Further numerical evidence for such bifurcations is presented in Fig. 13 where the discontinuity of sample III at \( T = .591 \) for the heating process is considered. In this figure the temperature variation of the free energy landscape is investigated by plotting the quantity

\[
f(T, v) = N^{-1}F(T, m_i \rightarrow m_i(T_c) + v u_i^{(0)}(T_c)). \tag{30}
\]

Below a critical temperature a minimum of the free energy and hence a stable solution exists in the region \( x > 0 \) which disappears by a saddle-node bifurcation above the critical temperature. Note that the stationary values of \( v \) determine approximately the temperature dependence of \( F \) near \( T_c \).

A further interesting detail is contained in Fig. 13. Below the critical temperature \( f \) is not semi-convex everywhere for \( x > 0 \), but above the critical temperature \( f \) is convex even in some regime \( x < 0 \). This demonstrates explicitly that the border of stability \( x = 0 \) is only approximative for finite systems.

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**FIG. 12: Saddle node bifurcation:** Smallest eigenvalue \( \lambda^{(0)} \) (dotted line), critical staggered magnetization \( \Delta m^{(0)} \) (full line) and an uncritical staggered magnetization \( \Delta m^{(1)} \) (dashed line) versus temperature \( T \) near the discontinuity at \( T_c = .6707 \) of Fig. 13. The dashed dotted line shows the leading behavior \( \Delta m^{(1)}(T) \sim (T_c - T)^2 \) near \( T_c \).

**FIG. 13: Free energy landscape:** Free energy density \( f = F/N \) versus distance \( v \) from the critical magnetization in direction of \( u^{(0)} \) for temperatures above and below the critical temperature \( T_c = .591 \) (compare text). Shown is the heating process of sample III for the state of lowest free energy. The stable solutions are indicated by dots. The full and the dashed lines correspond to the regimes \( x > 0 \) and \( x < 0 \), respectively.
IV. CONCLUSIONS

In this work we have demonstrated that the modified TAP equations are an adequate tool for exploring the characteristics of the pure states of the SK model of finite sizes. For all realizations of the random bonds explicit solutions exhibiting the spin glass features are obtained. Moreover, the present approach makes it possible to analyze the temperature dependence of all quantities of physical interest. In contrast to other approaches the method presented can simulate a slow cooling of the system, which is of particular importance to find the features of the low lying states.

Apart from these properties for the state of lowest free energy we have found some interesting statistical features of the meta stable states which seems to be generic for every sample and in the author’s opinion, it is a challenge to find an analytical approach to these features.

Due to finite size effects most of the results of this work are only qualitative. Thus systems of larger size should be investigated. This seems to be at least partially possible.

The present work uses a relaxational dynamics as a mathematical tool to find the pure states as fixpoints of the equations of motion. Recall that the origin of this dynamics is phenomenological and thus true dynamic effects cannot be described by the present approach. Thus the complete dynamical description should be a subject of further research.

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[22] Standard first order perturbation theory leads to $\lambda^{(0)} = B^{(0)} \Delta m^{(0)} \pm O(\Delta T)$ which implies the claimed result. Moreover $\lambda^{(0)} = \sqrt{\Delta T}$ holds for the stable branch in agreement with Fig.13.