Evidence for a Vanishing Complexity of the Sherrington-Kirkpatrick model

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Based on the modified Thouless-Anderson-Palmer equations a detailed numerical investigation for the complexity of the Sherrington-Kirkpatrick spin glass is worked out. The data suggest a scaling law which leads to a vanishing of the complexity in the thermodynamic limit as proposed recently. The results for the total number of stable states agree with existing approaches.

An important and common feature of all glassy systems with quenched disorder is the presence of a huge number \( N_s \) of stable or metastable thermodynamic states. This number typically grows exponentially

\[
N_s = \exp(N\Sigma^{\text{tot}}) \tag{1}
\]

with the size of the system \( N \) and determines the total complexity \( \Sigma^{\text{tot}} \). The number of states per free energy \( f \)

\[
N_s(f) = N_s \varrho_s(f) = \exp[N \Sigma(f)] = \sum_{\alpha=1}^{N_s} \delta(f - f_\alpha) \tag{2}
\]

defines both the normalized density \( \varrho_s(f) \) and the complexity \( \Sigma(f) \) where the \( f_\alpha \) are the values of the free energy per particle of the states labelled by \( \alpha = 1, \ldots, N_s \). The complexity or the density \( \varrho_s(f) \) characterize the organization of the thermodynamic states and is in addition expected to be of fundamental importance for an understanding of the dynamics in glasses [1].

The Sherrington-Kirkpatrick (SK) spin glass [2] is probably the simplest model to describe the physics of glasses. This model consists of \( N \) Ising spins connected to each other by the bonds \( J_{ij} \) which are independent random variables of variance \( N^{-1} \) with zero means. Computation of the complexity for the SK model were published more than two decades ago. The first was one presented by Bray and Moore (BM) [3]. Subsequent approaches basically equivalent to BM are given in [4]. In these early approaches a modulus sign of a Hessian determinant was dropped without any serious justification.

In a series of papers [5, 6, 7] this procedure has recently been criticized claiming that inadequacies and even inconsistencies result. Moreover such difficulties are also found for an alternative, the so-called Becci-Rouet-Stora-Tyutin (BRST) symmetric solution. Thus Crisanti et al. (CLPR) [7] proposed that no complexity occurs in the SK model. Contrary to the latter scenario Bray and Moore [8] and Aspelmeier et al. [9] have very recently presented new arguments for the validity of the BM approach and concluded that this theory remains a viable candidate for the spin glass complexity. Thus the analytical investigations of the complexity for the SK model are at present extremely controversial.

In this letter a numerical investigation of these problems is presented with the aim to clarify this controversy. Recalling that the thermodynamic states of the SK model are given by the solutions of the Thouless-Anderson-Palmer (TAP) equations [10], the method is obvious. Provided that the stable solution of these TAP equations and their associated free energies are known as function of the system size \( N \) it is just a simple counting and an extrapolation to the thermodynamic limit \( N \rightarrow \infty \) which has to be performed to find the distribution \( \varrho_s(f) \) and the total number of states \( N_s \).

The main difficulty is the explicit determination of the TAP states. A solution of this problem has recently been proposed by the present author [11]. This approach is based on a modification of the TAP equations which consistently describes both the stable solutions and the unstable solutions. Furthermore this approach employs a fictive dynamics to find the TAP solutions as fixed points of a set of equations of motion. These methods have been used to calculate successfully various physical quantities of the SK model [12]. Even some hints for behavior the complexity can be found in [12].

The latter methods are again used in the this work. Focusing exclusively on the complexity, the present investigation on this subject is much more detailed than [12]. As the main result of this letter, the numerical data demonstrate that the density \( \varrho_s(f) \) tends to a \( \delta \)-function

\[
\varrho_s(f) \rightarrow \delta(f - f_\text{eq}). \tag{3}
\]

in the thermodynamic limit which in agreement with the CLPR proposal implies that there is no complexity \( \Sigma(f) \) in the SK model. As a further result the numerical data suggest that the total complexity \( \Sigma^{\text{tot}} \) exists and is given by the BM theory. Thus both controversial approaches, the BM theory and CLPR proposal agree in parts with the present work although these approaches seem to be disjunct in the present form.

A vanishing complexity has interesting consequences. As all states have the same free energy value, none of them is thermodynamically preferred. Such a system is nothing else than a multi-phase system. The phase (or the mixture of phases) of any multi-phase system is generally selected by the (dynamic) history or by additional secondary interactions (like conjugate or symmetry breaking fields in conventional multi-phase systems). Note that these mechanisms are characteristic for glasses. Thus it should be possible to transfer at least some of the well understood techniques for conventional multi-phase systems to the SK spin glass.
After the presentation and the brief discussion of the main results, some more details are given in the remaining part of this letter. With reference to \[11\], \[12\] the essence of the modified TAP approach and of the numerical procedure is reviewed followed by the analysis of the numerical data.

In zero external field the modified TAP equations for the local magnetizations \( m_i = \langle S_i \rangle_\beta \) are given by the set of equations

\[
m_i = \tanh \beta \left\{ \sum_j J_{ij} m_j - m_i \chi_l \right\} \quad (4)
\]

with the local susceptibility

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

The quantity \( \Gamma \) is proportional to the density of zero eigenvalues of the inverse susceptibility matrix and is determined by

\[
\Gamma = 0 \quad \text{for} \quad x \geq 0 \quad (6)
\]

\[
1 = \frac{1}{N} \sum_i \frac{\beta^2 (1 - m_i^2)^2}{1 + \beta^2 (1 - m_i^2)^2} \quad \text{for} \quad x \leq 0 \quad (7)
\]

where

\[
x = 1 - \beta^2 (1 - 2q_2 + q_4) \quad (8)
\]

and where \( q_\nu = N^{-1} \sum_i m_i^\nu \ (\nu = 2, 4) \) it introduced. These equations are exact in the thermodynamic limit but can approximatively be used for large finite \( N \).

The condition \( x = 0 \) represents the central spin glass instability condition \[12\], \[14\], \[16\]. Above the instability \( (x \geq 0) \) the local susceptibility reduces to the isothermal value \( \chi_l = \beta (1 - q_2) \) and the Eqs.\[4\] are in complete agreement with the original TAP equations \[10\], \[15\]. Essential differences result below the instability \( (x < 0) \) as \( \Gamma > 0 \) and \( \chi_l \neq \beta (1 - q_2) \) hold for the modified TAP equations. This implies negative eigenvalues of the susceptibility matrix \[11\]. Thus all the states with \( x < 0 \) are unstable and have therefore no relevance for thermodynamic quantities for \( N \to \infty \).

For the stable states the free energy per spin \( f(\{m_i\}) \) is given by the well known expressions \[10\], \[12\]

\[
f(\{m_i\}) = -\frac{\beta}{2N} \sum_{i \neq j} J_{ij} m_i m_j - \frac{\beta^2}{4} (1 - q_2)^2 \quad (9)
\]

\[
+ \frac{1}{2} \sum \left\{ \frac{1 + m_i}{2} \ln \frac{1 + m_i}{2} + \frac{1 - m_i}{2} \ln \frac{1 - m_i}{2} \right\}
\]

from which the free energy values \( f_\alpha = f(\{m_\alpha^\alpha\}) \) of the TAP solutions \( \{m_\alpha^\alpha\} \quad (\alpha = 1, \ldots, N_s) \) are obtained.

The explicit calculation of these solutions \( \{m_\alpha^\alpha\} \) employs the relaxational Glauber dynamics

\[
m_i(t) = -m_i + \tanh \beta \left\{ \sum_j J_{ij} m_j - m_i \chi_l(t) \right\}. \quad (10)
\]

| \( N \) | \( N_{sys} \) | number of runs \( a \) | \( \Sigma^{tot} \) | \( w^x (\%) \) |
|---|---|---|---|---|
| 81 | 98 | 200 [25000] | 0.0545 | 7.5 |
| 100 | 57 | 1000 [5000] | 0.0552 | 7.5 |
| 120 | 27 | 1000 | 0.0512 | 8.6 |
| 150 | 25 | 150 [6000] | 0.0509 | 11.0 |
| 225 | 10 | 250 [29000] | (0.0428) \(^b\) | 10.8 |
| 400 | 6 | 250 [1000] | (0.0184) \(^c\) | 9.0 |
| 600 | 4 | 100 [400] | - | 6.7 |
| 800 | 2 | 120 | - | 7.7 |

\(^a\) The values in bracket apply only to one or two systems.
\(^b\) Average value calculated from 2 systems.
\(^c\) Lower bound for \( \Sigma^{tot} \) found in 1 system.

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where the local susceptibility \( \chi_l(t) \) is related to the \( m_i(t) \) via Eq.\[5\] and Eq.\[6\] or Eq.\[7\] depending on the instantaneous value of \( x(t) \). The fixed points solutions of Eqs.\[10\] coincide with the TAP solutions and both solutions exhibit identical stability properties \[12\]. Note that the phenomenological Eqs.\[10\] do not correctly describe dynamic effects (for microscopic equations of motion compare \[10\], \[17\]). They are, however, simple and are sufficient for the determination of the fixed point (or of the TAP) solutions.

The numerical procedure is analogous to the former work \[12\] to which the reader is referred for details. Again the integration routine ‘NDSolve’ of Mathematica on workstations is used to determine the \( \{m_\alpha^\alpha\} \) for a number of systems with different sizes as listed in Tab.\[I\]. All runs start with random initial conditions for the magnetizations \( \{m_\alpha^\alpha\} \) and nearly exclusively binary distributions of the bonds \( J_{ij} = \pm N^{-1/2} \) are used \[10\]. Although data for other temperatures are available the results presented are restricted to the temperature \( T = 0.2 \) following the previous work \[5\], \[6\], \[7\].

First the results for the total complexity \( \Sigma^{tot} \) are given which are (annealed) averages over \( N_{sys} \) systems. In Tab.\[I\] the obtained values are listed for sizes \( N \) up to 150 spins. The errors resulting from the system to system variations are found to be of the order of 10% . For \( N > 150 \) the numbers of runs are not sufficient to determine \( \Sigma^{tot} \) and at best some lower bounds can be given. From a strict point of view all values for \( \Sigma^{tot} \) are lower bounds as the applied procedure does not guarantee that all existing solutions are found. Based on investigations of some systems with a large number of runs, however, these errors can be estimated to be less than the uncertainty resulting from the system to system variations. For these estimates the decreases of the rate to find new solutions is analyzed when one increases the number of runs.

According to \[8\], the BM value and the BRST value for the complexity at \( T = 0.2 \) is given by \( \Sigma^{BM} = .0522 \) and
the histograms for the individual systems (labelled by $\Re$ lower bounds are given.

The latter conclusion even applies to those cases where only value but in disagreement with the BRST value. The $\Sigma$ temperature

law as described in the text.

Next the histograms corresponding to the densities $\Delta$ are analyzed. It is noted that all the shapes of the histograms for the individual systems (labelled by the index $n$) look similar and are nearly Gaussian. Thus histograms of the centered distributions

\[ P(v, N) = \langle \varphi_n^s(f^{n}_{av} + v) \rangle \]  
\[ f^{n}_{av} = \frac{1}{N^n} \sum_{\alpha} f_{\alpha} \]  

averaged over the $N_{sys}$ systems

\[ \langle \ldots \rangle = N^{-1} \sum_{n} \ldots \]  

are introduced and plotted in Fig.\textbf{1}. Without any doubt the plots exhibit a narrowing of the $P(v, N)$ with increasing values of $N$. Moreover this narrowing is compatible with the scaling law

\[ N^{-s} P(N, N^{-s}v) = \tilde{N}^{-s} P(\tilde{N}, \tilde{N}^{-s}v) = P(1, v) \]  

for arbitrary values of $N$ and $\tilde{N}$. With a deviation of less than one percent a standard numerical fitting leads to the value

\[ s = 1/3. \]  

Using for $P(1, v)$ a normalized Gaussian function with a standard deviation of 0.09117 the resulting fits are presented in Fig.\textbf{1} showing a good agreement with the histograms. Extrapolation of these results to $N \rightarrow \infty$ immediately leads to the main result of Eq. (3). Indeed the scaling law (13) implies $P(v, N) = N^{s} P(1, N^{s}v)$ which is a standard representation of the $\delta$-function.

The scaling relation (13) implies consequences for further quantities. Denoting the extremal values of the free energy of a specific system by $f_{min}$ and $f_{max}$ the widths defined by $\Delta = \langle f^{n}_{max} - f^{n}_{min} \rangle$ and by $\Delta_{2} = \langle f^{n}_{min} - f^{n}_{av} \rangle$ should vanish proportional to $N^{-s}$ in the thermodynamic limit. Indeed this dependence is found according to Fig.\textbf{1}.

Note that in this analysis no assumptions on the shapes enter which further supports the scaling relation.

Fig.\textbf{3} shows the minimum value of free energy $f_{min} = \langle f^{n}_{min} \rangle$ averaged over the $N_{sys}$ systems as function of $N^{-1/3}$. In the thermodynamic limit the width $\Delta_{2}$ vanishes. Thus the limiting value of $f_{min}$ for $N \rightarrow \infty$ equals the value $f_{eq}$ which arises in Eq. (4). By linear extrapolation the numerical value $f_{eq} = -0.7619$ is obtained which is in good agreement with the equilibrium value $-0.7594$ of the replica breaking approach at $T = 0.2$.

Some points of the above analysis need additional comments. Analogous to the findings of (12) the $x$ values of the majority of solutions are negative. Indeed according to Tab.\textbf{1} it is just a small fraction $w^{+}$ of the solutions which satisfy the condition $x > 0$. As discussed in (12) the solutions with $x < 0$ arise due to finite size effects and disappear with the power law $|x| \sim N^{-2/3}$ for $N \rightarrow \infty$ (compare Fig.2 of (12)). This behavior which also applies to the states with $x > 0$ and which is again found in the present approach is nothing else but the well known marginal stability of the TAP states in the thermodynamic limit. As shown in Fig.\textbf{1} both the states with $x > 0$ and the states with $x < 0$ are similar distributed.
Thus a separate analysis of the complexity is not needed for these two types of states.

Recall that for systems with large $N$ only a part of the TAP states can be determined and that only this part enters in the histograms of Fig.4. Therefore the interpretation of these histograms as $g_s(f)$ requires the assumption that this part of the states are representative for the set of all states. This assumption is checked for the systems where nearly all solutions are found. It is found that the first hundred runs give already reasonable approximations of the final results using several thousands runs. No significant changes result for the histograms, for the first hundred runs give already reasonable approximations of the final results using several thousands runs.

In particular there is no hint that the range of the free energies $\Delta_1$ increases to the BM value which is several times larger than the typical numerical values. Moreover according to BM results the number of these additional states should be large (a finite fraction of the total number of $N_s$). Thus a finite probability is expected to find at least some of these states which however is not the case. These arguments also apply if one takes in account that dynamical algorithms usually tend to prefer the states with lower free energy $\min f$. This effect is clearly observed in the present investigation. In disagreement to [9], however, it is concluded that this effect is not sufficiently distinctive to explain the huge differences to the BM approach.

Summing up, the numerical investigations demonstrate that the existing analytical approaches for the complexity of the SK model are at best partially valid. The present work strongly supports the CLPR proposal that there is no complexity for this model. Finally the scaling relation suggested by the numerical results may potentially be a guide for working out a consistent analytic theory.

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[1] G. Parisi, cond-mat/0301157
[2] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. 35 1972, (1975).
[3] A. J. Bray and M. A. Moore, J. Phys. C 13, L469 (1980).
[4] F. Tanaka and S. F. Edwards, J. Phys. F 10, 2471 (1980);
C. De Dominicis, M. Gabay, T. Garel and H. Orland, J. Physique 41, 923 (1980).
[5] A. Cavagna, I. Giardina, G. Parisi, and M. Mézard, J.
Phys. A 36, 1175 (2003); A. Annibale, A. Cavagna, I. Giardina, and G. Parisi, cond-mat/0304698
A. Annibale, A. Cavagna, I. Giardina, G. Parisi, and E. Trevigne, cond-mat/0307465
A. Crisanti, L. Leuzzi, G. Parisi, and T. Rizzo, cond-mat/0307543
A. Crisanti, L. Leuzzi, and T. Rizzo, cond-mat/0307586
A. Crisanti, L. Leuzzi, G. Parisi and T. Rizzo, cond-mat/0309256
[6] A. Crisanti, L. Leuzzi, G. Parisi, and T. Rizzo, cond-mat/0307082
[7] A. Crisanti, L. Leuzzi, G. Parisi, and T. Rizzo, cond-mat/0307586
[8] A. J. Bray and M. A. Moore, cond-mat/0305620
[9] T. Aspelmeier, A. J. Bray and M. A. Moore, cond-mat/0309113
[10] D. J. Thouless, P. W. Anderson, and R. G. Palmer, Phil.
Mag. 35, 593 (1977).
[11] T. Plefka, EuroPhys.Lett. 58, 892 (2002).
[12] T. Plefka, Phys. Rev. B 65, 224206 (2002). Two minor corrections of this work should be given: NIntegrate (third line of Sec.II D ) and 3850 (eighth line of Sec.III C) should be replaced by NDsolve and by 38500 respectively.
[13] J. R. L.de Almeida and D. J. Thouless , J. Phys. C: Solid State Phys., 11, 983 (1978).
[14] A. J. Bray and M. A. Moore, J. Phys. C: Solid State Phys. 12, L441 (1979).
[15] T. Plefka, J. Phys. A: Math. Gen., 15, 1971 (1982).
[16] T. Plefka, J. Phys. A: Math. Gen., 35, 8691 (2002).
[17] T. Plefka, cond-mat/0308172
[18] This averaging is used to reduces the finite size effects. According to the Figs.4 and 5 the system to system variations decrease with increasing $N$. This indicates the expected self averaging in the thermodynamic limit.
[19] For $N = 81$ a set of 28 systems with Gaussian distributions is included for which the values of ground state energy are exactly known [21]. Using an extrapolation from $T = 0.1$ the present algorithm finds 92% of the exact values within the first 50 runs. This efficiency is remarkable as it is expected that the ground state energy is missed in some cases due to saddle node bifurcations [12].
[20] C. M. Newman and D. L. Stein, Phys. Rev. E 60, 5244 (1999).
[21] S. Kobe, private communication (2003).

FIG. 3: Minimum value of free energy $f_{\min} = \langle f_{\min}^n \rangle$ versus $N^{-1}$ at a temperature $T = 0.2$. The length of each error bar is two standard deviations. The equilibrium value of the replica breaking approach is represented by the circle.