Modified TAP equations for the SK spin glass

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Abstract. – The stability of the TAP mean field equations is reanalyzed with the conclusion that the exclusive reason for the breakdown at the spin glass instability is an inconsistency for the value of the local susceptibility. A new alternative approach leads to modified equations which are in complete agreement with the original ones above the instability. Essentially altered results below the instability are presented and the consequences for the dynamical mean field equations are discussed.

Introduction. – Together with the replica approach, the Thouless-Anderson-Palmer (TAP) approach [1] is the most important method to analyze infinite range spin glass models like the Sherrington-Kirkpatrick (SK) model [2] of Ising spins (for reviews see [3, 4]). The TAP equations are well established [3–5] and are exact in the thermodynamic limit \( N \to \infty \) provided that the local magnetizations \( \{m_i\} \) satisfy the condition

\[
x \equiv 1 - \beta^2 (1 - 2q_2 + q_4) > 0 \quad \text{where} \quad q_\nu = N^{-1} \sum_i m_i^\nu \quad \nu = 2, 4.
\]

(1)

The condition (1) represents the central stability condition for the SK spin glass and therefore is also found in other approaches [3, 4, 6]. Within the TAP approach two different arguments for (1) are known. Bray and Moore [7] found a divergence of the spin-glass susceptibility for \( x \to 0 \). The expansion of Plefka [5], leading to the TAP equations, is limited to \( x > 0 \). In next section a further, basically simple, aspect of the stability condition is presented, leading naturally to a modification of the TAP equations.

Stability analysis revised. – The TAP free energy \( F \) of the SK model is given by

\[
F(\beta, \{m_i\}) = -\frac{1}{2} \sum_{ij} J_{ij} m_i m_j - \frac{N\beta}{4} (1 - q_2)^2 - \sum_i h_i m_i
\]

\[
+ \frac{1}{2\beta} \sum_i \left\{ (1 + m_i) \ln \frac{1 + m_i}{2} + (1 - m_i) \ln \frac{1 - m_i}{2} \right\}.
\]

(2)

where the \( \{h_i\} \) are local external fields. The bonds \( J_{ij} \) are independent random variables with zero means and standard deviations \( N^{-1/2} \). From \( \partial F/\partial m_i = 0 \) the TAP equations

\[
m_i = \tanh \beta \left\{ h_i + \sum_j J_{ij} m_j - \beta m_i (1 - q_2) \right\}
\]

(3)
result and the stability is governed by the inverse susceptibility matrix

\[
\chi_{ij}^{-1} = \partial h_i / \partial m_j = \partial^2 F / \partial m_i \partial m_j = \delta_{ij} \left\{ \beta^{-1} (1 - m_i^2)^{-1} + \beta (1 - q_2) \right\} - J_{ij}
\]

where the \( N^{-1} \)-order term \(-2N^{-1} \beta m_i m_j \) has been dropped as it has no influence on the present analysis (compare, however, \( \text{[3]} \) and the footnote below).

According to (2), the free energy is formally well defined for all values of the \( \{m_i\} \) inside the hyper cube \(|m_i| \leq 1 \) including the regime \( x < 0 \). The question is which physical requirement is violated for \( x < 0 \). To answer this question we investigate the free energy for convexity, a fundamental requirement for every free energy function. This can be done without explicit knowledge of the solutions of (3). The analysis is performed analogously to \( \text{[5]} \) and the resolvent of the matrix \( \chi^{-1} \) is introduced

\[
R(z) \equiv N^{-1} \text{Tr} (z - \chi^{-1})^{-1}.
\]

It is important to note (compare appendix) that \( R(z) \) is an element of the class of functions which are analytic in \( z \) for \( \text{Im} z \neq 0 \) and such that

\[
\text{Im} R(z) > 0 \quad \text{for} \quad \text{Im} z < 0.
\]

The key for further analysis is the powerful theorem of Pastur \( \text{[8]} \), rederived in \( \text{[7]} \) as ‘locator expansion’. According to (22) the resolvent \( R(z) \) satisfies the equation

\[
R(z) = N^{-1} \sum_i \left\{ z - R(z) - \beta^{-1} (1 - m_i^2)^{-1} - \beta (1 - q_2) \right\}^{-1}
\]

in the \( N \to \infty \) limit for nearly all configurations of the bonds (which does not imply averaging). Eq. (২) is basically a polynomial of the order \( N + 1 \) and has therefore \( N + 1 \) solutions for \( R(z) \). With reference to the appendix and to \( \text{[3]} \), however, there is only one solution which satisfies (3). Thus \( R(z) \) can uniquely be determined.

Near \( x = 0 \) and \( z = 0 \), the leading behavior of \( R(z) \) is obtained by a power expansion of the right hand site of (২) in terms of \( \{R - z + \beta (1 - q_2)\} \). To second order

\[
p \left\{ R - z + \beta (1 - q_2) \right\}^2 + x \left\{ R - z + \beta (1 - q_2) \right\} + z = 0
\]

is found, where \( p = \beta^3 N^{-1} \sum_i (1 - m_i^2)^3 \) is a positive quantity. For the case \( p|z| \ll x^2 \), the solutions \( R^\pm(z) \) are given by

\[
\{R^+ - z + \beta (1 - q_2)\} = -z / x \quad \text{and by} \quad \{R^- - z + \beta (1 - q_2)\} = -x / p + z / x
\]

where according to the requirement (3) the solution \( R^+(z) \) applies for \( x > 0 \) and the solution \( R^-(z) \) applies for \( x < 0 \), respectively.

Several important conclusions can be made. According to (৫)

\[
\chi_l \equiv -\text{Re} R(z) \bigg|_{z \to 0} = N^{-1} \text{Tr} \chi
\]

holds for the local susceptibility \( \chi_l \), which gives, with eq. (৫)

\[
\chi_l = \beta (1 - q_2) \quad \text{for} \quad x > 0 \quad \text{and} \quad \chi_l = \beta (1 - q_2) + x / p \quad \text{for} \quad x < 0,
\]

respectively. The value of \( \chi_l \) deviates from the value \( \beta (1 - q_2) \) for \( x < 0 \). The latter value, however, is exact for an arbitrary Ising model in the canonical distribution as can easily be
shown. Moreover, in general, the exact value is used at the beginning of the derivations leading to the TAP equations. Thus the inconsistent result $\chi_l \neq \beta (1 - q_2)$ causes the breakdown of the TAP approach for $x < 0$.

The spin glass susceptibility $\chi_{sg}$ is, according to (5), related to $R(z)$ by

$$\chi_{sg} \equiv -\text{Re} \left( \frac{\partial R(z)}{\partial z} \right) \bigg|_{z \to 0} = N^{-1} \text{Tr} \chi^2$$

from which in leading order

$$\chi_{sg} = |x|^{-1} \quad (x \neq 0)$$

is obtained. Apart from the divergence, $\chi_{sg}$ is well behaved and positive everywhere. The earlier work [4,7] is therefore restricted to the case $x > 0$, although this is not explicitly stated.

Within the replica method $\chi_{sg}$ becomes negative for $x < 0$ [3,4]. According to (9), a negative $\chi_{sg}$ only results if (6) is violated.

The eigenvalue density $\varrho(\lambda)$ of $\chi^{-1}$ is determined from $R(z)$ by

$$\varrho(\lambda) = \frac{\pi}{2} \left| \text{Im} R(\lambda - i\epsilon) \right|_{\epsilon \to 0^+} .$$

With the full solution of the quadratic eq.(13) one obtains for small values of $\lambda$ and of $x$

$$\varrho(\lambda) = \pi^{-1} p^{-1/2} \sqrt{\lambda - x^2/p}. \quad (15)$$

This result shows that the minimum eigenvalue of $\chi^{-1}$ is given to leading order by

$$\lambda_{\text{min}} = x^2/p \geq 0 \quad \text{for} \quad |x| \to 0. \quad (16)$$

With the extension to arbitrary values of $x$ given in the appendix, the last result implies that negative eigenvalues do not occur and the TAP free energy is semi-convex everywhere. Note that the present analysis and thus the results are limited to the leading order in $N$. Hence the TAP free energy may not be semi-convex everywhere on sub-extensive scales. Such an interesting behavior was found for the p-spin spherical model [9] and is expected in regions near $x = 0$ due to finite size effects of $\varrho(\lambda)$.

The modified TAP equations. – It was shown that the TAP equations break down for $x < 0$ due to an inconsistency for the value of $\chi_l$. We therefore look for modified equations which do not show such an unsatisfactory behavior. The present analysis starts with the well founded expressions [1,3,4] which are rederived in the appendix

$$m_i = \tanh \beta \{ h_i + \sum_j J_{ij} m_j - m_i \chi_l \} \quad (17)$$

where the local susceptibility is given by $\chi_l = N^{-1} \sum_i \chi_{ii} = N^{-1} \sum_i \partial m_i / \partial h_i$. With the working hypothesis that $\partial \chi_l / \partial m_i$ is a order $N^{-1}$ term, the inverse susceptibility matrix $\chi_{ij}^{-1}$ is calculated from eqs.(17) to

$$\chi_{ij}^{-1} = \delta_{ij} \left\{ \beta^{-1} (1 - m_i^2)^{-1} + \chi_l \right\} - J_{ij}. \quad (18)$$

(1) In this context the sub-extensive terms to $\chi^{-1}$ neglected in eq. [1] and leading to a second stability condition $1 - 2\beta^2 (q_2 - q_4) > 0$ (compare [4]) may have some effect despite the conclusions of [10] that these terms are not important.
Note that the eqs. (17), (18) and \( \sum \chi_{ij} \chi^{-1}_{jk} = \delta_{ik} \) represent a closed set of self consistent equations for the \( m_i \), the \( \chi_{ij} \) and the \( \chi^{-1}_{ij} \). This fact is the key to the present approach. Moreover it is important to realize that already the eqs. (17) are complete and sufficient to determine all solutions as the eqs. (18) result from eqs. (17). In this context the restriction of the original TAP equations to \( x > 0 \) is obvious as the replacement \( \chi_l \to \beta(1-q_2) \) is only justified for stable solutions but will lead to inconsistencies for other solutions.

The theorem of Pastur leads to a very effective simplification of the above set of equations. Application of this theorem yields \( R(-i\epsilon) = -N^{-1} \sum \{ \beta^{-1}(1-m_i^2)^{-1} + R(-i\epsilon) + \chi_l + i\epsilon \}^{-1} \) where \( R(z) \) is now related to \( \chi^{-1} \) given in eq. (18). Performing the limit \( \epsilon \to +0 \), taking again care of the requirement (6), noting that \( \chi_l = -\text{Re} R(-i\epsilon) |_{\epsilon \to +0} \) holds and separating the real and imaginary parts finally results in

\[
\chi_l = \frac{1}{N} \sum_i \frac{\beta(1-m_i^2)}{1 + \Gamma^2 \beta^2(1-m_i^2)^2} \quad \text{for } x \geq 0 \quad (19) \\
1 = \frac{1}{N} \sum_i \frac{\beta^2(1-m_i^2)^2}{1 + \Gamma^2 \beta^2(1-m_i^2)^2} \quad \text{for } x \leq 0 \quad (20)
\]

where \( \Gamma = \pi^{-1} \rho(0) = \text{Im} R(-i\epsilon) |_{\epsilon \to +0} \geq 0 \) was introduced. Note that both \( \chi_l \) and \( \Gamma \) are continuous at \( x = 0 \) and note the latter eq. of (20) has always a solution \( \Gamma \) for \( x < 0 \). Finally it is easy to show that the above working hypothesis is satisfied.

The set of eqs. (17), (19) and (20) represent the modified TAP equations which determine \( \{ m_i \}, \chi_l \) and \( \Gamma \) for all temperatures and all magnetic fields. In the region \( x > 0 \), the modified and the original TAP equations and thus their solutions are identical. Dramatic changes, however, are found for the region \( x < 0 \) in which the equations differ, leading in general to different solutions. The stability of the solutions is governed by the value of \( \Gamma \) which is proportional to the eigenvalue density \( \rho(0) \). In the region \( x > 0 \) all solutions are stable with \( \Gamma = 0 \) and in the regime \( x < 0 \) all solutions are unstable with \( \Gamma > 0 \).

A solution of special interest is the paramagnetic solution \( m_i = 0 \) in zero field. This solution satisfies the modified TAP equations with \( \Gamma = (1-T^2)^{1/2} > 0 \) for \( T < 1 \) and with \( \Gamma = 0 \) for \( T > 1 \), respectively. Thus the solution is unstable for temperatures below \( T = 1 \). This physically important result is not found by the original TAP approach which gives a stable paramagnetic solution for all temperatures.

Eq. (13) shows that for all stable solutions the value of \( \chi_l \) equals the thermodynamic value \( \beta(1-q_2) \). A difference of these two values occurs for the unstable solutions. This is not in conflict with thermodynamics which is a priori limited to stable states.

The last argument, the general limitation of equilibrium thermodynamics to stable states, implies that for unstable states thermodynamic functions like the entropy or the free energy are not defined \(^{(2)}\). Again from the strict thermodynamic point of view the original and the modified TAP equations are equivalent as both lead to the same results for the stable states. It is the reason for the breakdown which differs in both approaches. The inconsistency for \( \chi_l \) for \( x < 0 \) of the original TAP equations is rather unconventional compared to the modified equations where the usual behavior, negative eigenvalues of \( \chi^{-1} \), applies.

Unstable states are important for phenomenological extensions to dynamics. On basis of the modified TAP equations and in contrast to the usual TAP treatment such a phenomenological but consistent extension to the dynamics becomes possible. In analogy to \( ^{(1)} \) the relaxational Glauber dynamics in mean field approximation will be used for this purpose.

\(^{(2)}\) Discussions based on free energy landscapes use often extensions of thermodynamic free energies to the unstable regimes. Thus such approaches are phenomenological. For the present work such an obvious extension is not available and the basically equivalent approach via relaxational equations of motions is employed.
Fig. 1 – Zero field solution of the modified TAP equations. (a) Edwards Anderson parameter $q_2$ (full line), $x \equiv 1 - \beta^2(1 - 2q_2 + q_4)$ (dotted line), $\Gamma$ (dashed line), (b) free energy density $f = F/N$ (full line) and entropy density $s$ (dashed line) versus temperature $T$ for a system with $N = 100$ and with $J_{ij} = \pm N^{-1/2}$. The solution is obtained from the integration of (21) by slowly cooling down from $T = 1$. The discontinuities at $T = .078$ and $T = .551$ result from saddle-node bifurcations with jumps to lower values of $f$ (which are not resolved on the scale of (b)). Slow heating leads to hysteresis effects near the discontinuities.

Measuring the time in units of the relaxation time, the equations of motion are given by

$$\dot{m}_i(t) = -m_i(t) + \tanh \beta \{ h_i + \sum_j J_{ij} m_j(t) - m_i(t) \chi_i(t) \}$$

(21)

where $\chi_i(t)$ again is determined by eqs. (19) and (20). The fixpoints of (21) coincide with the solutions of static equations and a one-to-one correspondence between the dynamical stability of the fixpoints and the thermodynamic stability holds. Moreover the eqs. (21) simulate the evolution of thermodynamic processes in which $\beta$ or $h_i$ are changed. Using the initial magnetizations of such a process as initial values for the time integration, the system relaxes to a stable fixpoint which corresponds to a stable solution of the static TAP equations and thus to the final state of the thermodynamic process. The dynamical approach uniquely determines the final state even in those cases where the system exhibits meta- or multi-stability. From the pure knowledge of the static solutions such a determination of the final state is not possible.

The final states are stable and thus they are always located outside the regime $x < 0$. During the dynamic evolution, however, the system may temporarily stay or may even start in the region $x(t) < 0$. Thus the flow of eq. (21) is needed in both regions $x(t) > 0$ and $x(t) < 0$. These arguments demonstrate the relevance of the unstable states. Note that equations of motion of the above type but based on the original TAP equations usually lead to incorrect results in the spin-glass regime as the system relaxes to paramagnetic solutions.

As the eqs. (21) are phenomenological they do not describe the true dynamical effects of the SK model but can be used as a numerical tool to find explicitly the solutions of the TAP equations for finite $N$. Numerical work which is based on this method and which is an alternative approach to [12], will be published separately [13].

To demonstrate that this method is successful some results of [13] are presented in fig. (1). A system of $N = 100$ spins with $h_i = 0$ and with binary distributions of the $J_{ij}$ was investigated. By numerical integration of eqs. (21) with (19) and (20) the fixpoints of these equations have been calculated in the temperature range from $T = 1$ down to $T = .01$ with a step size of
\[ \delta T = 0.01. \] The first run at \( T = 1 \) has performed with the initial values \( m_i = 0 \). All other runs use as initial values the fixpoint values of the former run to simulate a slowly cooling down. The results for \( q_2, x, \Gamma \), the free energy and the entropy density are plotted in fig. (1). Due to finite size effects the boundary for the stability \( x = 0 \) is not exact for finite \( N \). Thus as shown in fig. (1) stable fixpoint solutions with \( \Gamma > 0 \) and with \( x < 0 \) are found. With increasing \( N \), however, the boundary for stability tends to \( x = 0 \) as demonstrated in (13).

**Conclusions.** Based on a careful stability analysis it has been worked out that the TAP equations need a modification in the region of instability. This modification leads to a complete and consistent description of the spin glass instability including the unstable region. Although the new, unstable states cannot be observed, the unstable regime essentially determines the flow of the equation of motion and thus affects the basins of attraction of the stable states.

The semi-convexity of the TAP free energy in the thermodynamic limit represents a further result of importance as it implies that the 'multi-valley' structure of the TAP free energy occurs on a sub-extensive scale. For further investigations of these important effects the modified equations are expected to be an adequate tool. It is straightforward to extend the analysis from the SK model to the other numerous spin glass models of infinite range and results similar to those of the present work are expected.

**Appendix:** In the first point in this section eq. (17), which is the starting point for the derivation to the modified TAP equations is redervied. Similar to the approaches in the SM the \( N - 1 \) spin system is considered, with the Ising spin \( S_n \) removed from the \( N \) spin system under investigation. Taking the trace over the spin \( S_n \) leads to the exact relations for all \( i \neq n \)

\[ m_i = \hat{m}_i + \frac{1 + m_n}{2\beta} \frac{\partial a_n^+}{\partial h_i} + \frac{1 + m_n}{2\beta} \frac{\partial a_n^-}{\partial h_i} \quad , \quad m_n = \frac{\exp(a_n^+ + \beta h_n) - \exp(a_n^- - \beta h_n)}{\exp(a_n^+ + \beta h_n) + \exp(a_n^- - \beta h_n)} \]

where \( \hat{m}_i = \langle S_i \rangle_{N-1} \) and \( \exp(a_n^\pm) = \langle \exp(\pm \beta \sum J_{ni} S_i) \rangle_{N-1} \) are expectation values of the \( N - 1 \) spin system. Note that latter of these values can be rewritten as a ratio of two partition functions with fields \( h_i \pm J_{ni} \) and with fields \( h_i \), respectively. With the remark that the next steps are only justified to the leading order in \( N^{-1} \) one finds by a cumulant expansion \( a_n^\pm = \pm \beta \sum J_{ni} \hat{m}_i + \beta \sum_{ij} J_{ni} J_{nj} \partial \hat{m}_i / \partial h_j \). This leads to eq. (17) with \( \chi_i = \sum_{ij} J_{ni} J_{nj} \partial \hat{m}_i / \partial h_j \) which can to leading order be approximated to \( \chi_i = N^{-1} \sum_i \partial \hat{m}_i / \partial h_i \) due to the random character of the \( J_{ni} \).

The theorem of Pastur [3] is central for the present work and in the remaining part of this appendix two technical aspects related to this theorem are worked out. Let \( K_{ij} = k \delta_{ij} \) be a non-random matrix in \( N \) dimensional space with all \( k \) real valued and let \( J_{ij} \) be a symmetric matrix (with \( J_{ij} = 0 \), where the off-diagonal elements are independent random quantities with zero means and standard deviations \( N^{-1/2} \). According to this theorem the resolvent \( R(z) = N^{-1} \text{Tr} \{ z - K + J \}^{-1} \) satisfies the equation in the limit \( N \to \infty \)

\[ R(z) = N^{-1} \text{Tr} \{ z - K - R(z) \}^{-1} = N^{-1} \sum_i \{ z - k_i - R(z) \}^{-1}. \] (22)

Focusing on the properties of the \( N + 1 \) solutions of \( f(x) = N^{-1} \sum_k \{ k_i + x \}^{-1} \) is introduced and \( k_1 < k_2 \ldots < k_N \) is presumed. Setting \( r = R(z = 0) \), the solutions of \( f(x) \) for the case \( z = 0 \) are determined by \( -r = f(r) \). According to fig. (3) there are always \( N - 1 \) real solutions \( r_i \) \(( \sim k_i ) \) for \( i = 2, \ldots , N \). Depending on the values of \( k_i \) two cases are possible for the two remaining solutions: For case (i) both solutions are real and will be denoted by \( r_1 \) and \( r_0 \) (with \( r_1 < r_0 \)). For case (ii) a pair of conjugate complex solutions \( c^\pm \) results with Im \( c_+ > 0 \) and with Im \( c_- < 0 \), respectively.
leads to the identity (22) while the latter can be obtained by a discussion similar to fig.(2). The definition of the solutions of $\bar{r}$ focusing to the original TAP case $k$ may be absent depending on the values of the $k_i$.

Fig. 2 – Graphical solution of the equation $-\tau = N^{-1} \sum_i (r + k_i)^{-1} \equiv f(r)$. The solutions $r_0$ and $r_1$ may be absent depending on the values of the $k_i$.

In the next step the linear terms in $z$ of the solutions $R_i(z)$ of (22) are calculated by expansion for $|z| < 1$ near the real solutions $r_i$. The ansatz $R_i(z) = r_i + a_i z$ leads in linear approximation to $-r_i - a_i z = f(r_i + a_i z - z) \approx f(r_i) + f'(r_i)(a_i - 1) z$ from which $a_i = f'(r_i)(1 + f'(r_i))^{-1}$ results. Fig.(4) shows, that $-1 < f'(r_0) < 0$ and $f'(r_{i\neq 0}) < -1$ holds and in consequence $a_0 < 0$ and $a_{i\neq 0} > 0$ results. Thus with the secondary requirement Im $R(z) > 0$ for Im $z < 0$, the solution of (22) is unique determined and given in the limit $z \to 0$ by $r_0$ in case (i) and by $c_i$ in case (ii), respectively. The definition of $R(z)$ satisfies this requirement as Im $R(z) = -N^{-1} \text{Im} z \sum_i \{ (\Lambda + \text{Re} z)^2 + (\text{Im} z)^2 \}^{-1}$ holds, where $\Lambda$ are the real eigenvalues of $-K + J$. Thus the solution of (22) together with the requirement (ii) determines $R(z)$ uniquely.

Let us finally consider the special points $\hat{\lambda}$ on the real axis in the $z$ plane where the real solutions $R(\hat{\lambda}) = \hat{r}$ of (22) bifurcate to complex values. The values $\hat{\lambda}$ and $\hat{r}$ are determined by the solutions of $\hat{r} = -f(\hat{r} - \hat{\lambda})$ and of $f'(\hat{r} - \hat{\lambda}) = -1$. The first equation is just the theorem (22) while the latter can be obtained by a discussion similar to fig.(4). The definition of $f(x)$ leads to the identity $f(u) - f(v) + (v - u)f'(v) = N^{-1}(v - u)^2 \sum_i (k_i + u)^{-1}(k_i + v)^{-2}$. Focusing to the original TAP case $k_i = \beta^{-1}(1 - q_i^2)^{-1} + \beta(1 - q_2)$ has to be used according to (4) and (24). Setting $u = -\beta(1 - q_2)$ and setting $v = \hat{r} - \hat{\lambda}$ the identity and the above equations lead to the important result $\hat{\lambda} \geq 0$. This result implies that all endpoints of the intervals with a finite $\rho(\lambda)$ are located on the positive axis. A $1/z$ expansion of (4) shows that $\rho(\lambda) \equiv 0$ for large negative $\lambda$. Thus the minimum eigenvalue satisfies $\lambda_{\text{min}} \geq 0$ which generalizes the result (4) to all values of $x$.

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