Role of free energy landscape in the dynamics of mean field glassy systems

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In this paper we expose the results of our recent work on the dynamical TAP approach to mean field glassy systems. Our aim is to clarify the connection between free energy landscape and out of equilibrium dynamics in solvable models.

Frequently qualitative explanations of glassy behaviour are based on the “Free Energy Landscape Paradigm”. If its relevance for equilibrium properties is clear, the relationship between free energy landscape and out of equilibrium dynamics is not well understood yet. In this paper we clarify this relationship for the class of spin glass models which reproduce phenomenologically some features of structural glasses. The method we use is a generalisation to dynamics of the Thouless, Anderson and Palmer approach to thermodynamics of mean field spin glasses. Within this framework we show to what extent the dynamics can be represented as an evolution in the free energy landscape. In particular the relationship between the long-time dynamics and the local properties of the free energy landscape shows up explicitly using this approach.

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I. INTRODUCTION

Generally in the study of thermodynamics much attention is payed to the free energy landscape [1]. This landscape, which can be interpreted as the effective potential whose minima represent different possible states, gives an intuitive and quantitative description of the equilibrium properties. Consider for example ferromagnetic systems. In this case the effective potential is a function of magnetisation. The ferromagnetic transition corresponds to the splitting of the paramagnetic minimum in the two ferromagnetic minima. At low temperature a vanishing external magnetic field breaks the up-down symmetry and fixes the system in one of the two possible ferromagnetic states.

Generally, glassy systems are characterised by a complicated energy landscape, which can give rise eventually to the existence of many possible states. Frequently, qualitative explanations of glassy behaviours are based on some assumptions on the properties of the free energy landscape [1]. Consider for example the Kirkpatrick-Thirumalai-Wolynes scenario for the glass transition [2,3] in which the (exponential) number of states with a given free energy plays a crucial role.

However, if the relevance of the free energy landscape for the equilibrium properties is clear, the relationship between the free energy landscape and the dynamical behaviour is not completely understood, especially for glassy systems which remain out of equilibrium also at long time. For instance what we can learn on the (out of equilibrium) dynamical behaviour starting from the knowledge of the free energy landscape is not clear.

All the explanations based on the free energy landscape remain often at a qualitative level, because in general this landscape cannot be computed and studied exactly. Only for mean field frustrated systems this “Landscape Paradigm” [1] has received a firm theoretical basis. In this case an analytic solution of the thermodynamics [4] and of the asymptotic out of equilibrium dynamics [5] is available. For these systems the free energy landscape can be computed [6] [7] and the partition function, and therefore the equilibrium properties, can be recovered as a sum over the free energy minima weighted with the Boltzmann factor [8]. This approach to the thermodynamics of mean field spin glasses is called the TAP approach, because it was introduced by Thouless, Anderson and Palmer for the Sherrington-Kirkpatrick model [13]. In this paper we focus on the class of spin glass models which reproduce phenomenologically some features of structural glasses [4] [9]. To understand the relationship between free energy landscape and dynamical behaviour we generalise the TAP approach to dynamics.

II. THE TAP APPROACH

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A. Static TAP equations

In the following we show how the free energy landscape, also called TAP free energy, can be derived for the p-spin spherical model. The aim of this section is to present in a simple case the strategy which we have followed to compute the dynamical TAP equations. The p-spin Hamiltonian reads:

\[ H(\{S_i\}) = - \sum_{1 \leq i_1 < \ldots < i_p \leq N} J_{i_1,\ldots,i_p} S_{i_1} \cdots S_{i_p} \]  

where the couplings are Gaussian variables with zero mean and average \( \overline{J_{i_1,\ldots,i_p}^2} = \frac{\beta}{2N^p} \). The TAP free energy \( \Gamma(\beta, m_i, l) \), which depends on the magnetisation \( m_i \) at each site \( i \) and on the spherical parameter \( l \), is the Legendre transform of the “true” free energy:

\[ -\beta \Gamma(\beta, m_i, l) = \ln \int_{-\infty}^{+\infty} \prod_{i=1}^{N} ds_i \exp \left( -\beta H(\{S_i\}) - \sum_{i} h_i(S_i - m_i) - \frac{\lambda}{2} \sum_{i=1}^{N} (S_i^2 - l) \right) \]  

The Lagrange multipliers \( h_i(\beta) \) fix the magnetisation at each site \( i \): \( \langle S_i \rangle = m_i \) and \( \lambda(\beta) \) enforces the condition \( \sum_{i=1}^{N} \langle S_i^2 \rangle = N \). \( \langle \cdot \rangle \) denotes the thermal average and \( N \) is the number of spins.

Once \( \Gamma \) is known, the equation \( -\frac{\partial \Gamma}{\partial m_i} \bigg|_{l=1} = h_i \) fixes the spherical constraint \( \sum_{i} S_i^2 = N \) and gives the spherical multipliers as a function of \( m_i \), whereas \( -\frac{\partial \Gamma}{\partial m_i} \bigg|_{l=1} = h_i \) are the TAP equations, which fix the values of local magnetisations.

The standard perturbation expansion for the generalised potential \( \Gamma \) is rather involved and cannot be directly applied to the Ising case. Thus, we prefer to follow the approach developed for the Sherrington-Kirkpatrick model by T. Plefka and A. Georges and S. Yedidia because it is simple and can be directly applied to all mean field spin glass models. They obtained the TAP free energy for the Sherrington-Kirkpatrick model expanding \( -\beta \Gamma \) in powers of \( \beta \) around \( \beta = 0 \). For a general system this corresponds to a \( \frac{1}{d} \) expansion (\( d \) being the spatial dimension) around mean field theory; so it is not surprising that for mean field spin glass models only a finite number of terms survives. The zeroth- and first-order terms give the “naive” TAP free energy, whereas the second term is the Onsager reaction term.

From the definition of \( -\beta \Gamma \) given in equation (2), we find that the zeroth-order term is the entropy of non interacting spherical spins constrained to have magnetisation \( m_i \):

\[ -\beta \Gamma(\beta, m_i, l) \bigg|_{\beta=0} = \frac{N}{2} \ln \left( l - \frac{1}{N} \sum_{i=1}^{N} m_i^2 \right) \]  

Using the Lagrange conditions and that the spins are decoupled at \( \beta = 0 \) we find that the linear term in the power expansion of the TAP free energy equals:

\[ -\beta \frac{\partial (\beta \Gamma)}{\partial \beta} \bigg|_{\beta=0} = \frac{\beta}{2} \sum_{1 \leq i_1 < \ldots < i_p \leq N} J_{i_1,\ldots,i_p} m_{i_1} \cdots m_{i_p} \]  

This “mean field” energy together with the zeroth-order term gives the standard mean field theory, which becomes exact for infinite-ranged ferromagnetic system. The Onsager reaction term comes from the second derivative of \( \Gamma \):

\[ -\frac{\beta^2}{2} \frac{\partial^2 (\beta \Gamma)}{\partial \beta^2} \bigg|_{\beta=0} = \frac{\beta^2}{2} \left( \left( \sum_{1 \leq i_1 < \ldots < i_p \leq N} Y_{i_1,\ldots,i_p} \right)^2 \right)_{\beta=0} \]  

\(^1\)We are neglecting a useless additive constant in \( \Gamma \). A term in \( \Gamma \), that does not depend on \( l \) and \( m_i \), has no influence on thermodynamics.
\[ Y_{i_1, \ldots, i_p} = J_{i_1, \ldots, i_p} S_{i_1} \cdots S_{i_p} - (S_{i_1} - m_{i_1}) m_{i_2} \cdots m_{i_p} - \cdots - m_{i_1} \cdots m_{i_{p-1}} (S_{i_p} - m_{i_p}) . \]

To compute (8) we have used the following Maxwell relations:

\[
\begin{align*}
\frac{\partial h_i}{\partial \beta} \bigg|_{\beta=0} &= - \frac{\partial}{\partial m_i} \left( \frac{\partial \Gamma}{\partial \beta} \right) \bigg|_{\beta=0} \\
\frac{\partial \lambda}{\partial \beta} \bigg|_{\beta=0} &= - 2 \frac{\partial}{\partial m_l} \left( \frac{\partial \Gamma}{\partial \beta} \right) \bigg|_{\beta=0}
\end{align*}
\]

Using the statistical properties of the couplings it is easy to check that the only terms giving a contribution of the order of \( N \) correspond to the squares of \( J_{i_1, \ldots, i_p} \):

\[
- \frac{\beta^2}{2} \frac{\partial^2 (\beta \Gamma)}{\partial \beta^2} \bigg|_{\beta=0} = \frac{\beta^2}{2} \sum_{1 \leq i_1 < \cdots < i_p \leq N} \left\langle Y_{i_1, \ldots, i_p} \right\rangle^c \bigg|_{\beta=0} .
\]

Using again the statistical properties of the couplings and neglecting terms giving a contribution of an order smaller than \( N \) we find that the reaction term depends on \( m_i \) through the overlap \( q = \frac{1}{N} \sum_i m_i^2 \) only:

\[
- \frac{\beta^2}{2} \frac{\partial^2 (\beta \Gamma)}{\partial \beta^2} \bigg|_{\beta=0} = \frac{\beta^2 N}{4} (l^p - q^p - p(1q^{p-1} - q^p)) .
\]

Higher derivatives lead to terms which can be neglected because they are not of the order of \( N \); so collecting (8), (9) and (6) we find the TAP free energy for spherical p-spin models. Differentiating the free energy with respect to magnetisations \( m_i \) and the spherical parameter \( l \) one finds the TAP equations. These equations admit for certain temperatures an infinite number of solutions. This is a fundamental characteristic and difficulty of mean field spin glasses.

It has been shown \[12\] that the weighted sum of the local minima of the TAP free energy gives back equilibrium results found by the replica or the cavity method \[8\]: \( Z = \sum_{\alpha} e^{-N f_{\alpha}} \), where \( f_{\alpha} \) is the TAP free energy of a stable solution \( \{ m_i^\alpha \} \) of TAP equations. Note that states which do not have the minimum free energy can dominate the previous sum if their number is very large.

Let us conclude this section with few comments on the derivation of the static TAP equations. First of all we remark that we have improperly called \( \Gamma(\beta, m_i, l) \) a Legendre transform. Indeed the function \( \Gamma(\beta, m_i, l) \) is the generating functional of proper vertices \[17\]. This function may have many minima and is not convex in general. Finally we want to point out a striking difference, which arises in the computation of \( \Gamma \) between completely connected and finite connectivity mean field models. For the former the expansion of \( \Gamma \) in powers of \( \beta \) stops at the second order in \( \beta \). Whereas for the latter the expansion contains all the powers of \( \beta \). Roughly speaking for the Sherrington-Kirkpatrick model the only non trivial term in \( \Gamma \) is the reaction term, which represents the contribution to the effective field of the \( i \)th spin due to the influence of the \( i \)th spin on the others. Whereas for its counterpart on a Bethe lattice \[8,11\] the interaction between two neighbouring spins has to be taken into account exactly, i.e. one has to take into account not only the reaction of the neighbours of \( S_i \) due to the presence of \( S_i \), but also the reaction of the reaction and so on.

### B. Dynamical TAP equations

In the following we focus on a Langevin relaxation dynamics for mean field glassy systems. Standard field theoretical manipulations \[17\] lead to the Martin-Siggia-Rose generating functional for the expectation values of \( s_i(t) \).

Within the superspace notation \[17,19\] the dynamics and the static theory are formally very similar \[19\]. As a consequence dynamical TAP equations can be derived straightforwardly generalising the method described in the previous section. We refer to \[17\] for a detailed derivation. Once the dynamical TAP free energy is known, the dynamical TAP equation are obtained from the Lagrange relation for the supermagnetisation. In the following we simply quote the result \[17\]:

3
where \( h_{t} \) to magnetic fields average over all possible configurations as in [20], then the magnetisations are equal to zero at \( \langle \cdot \rangle \), that now because it represents the contribution to the effective field of the gradient descent in the free energy landscape since the Onsager reaction term is non-Markovian. This is natural limit the equation (12) coincides with a simple gradient descent, as should be when the thermal noise is absent.

Two asymptotic behaviour have been found for the p-spin spherical model depending on the choice of the initial conditions (15) says.

In the following we perform an asymptotic analysis of the equations (10), (11), (12) and (13). For the sake of simplicity we will take \( h_{i}(t) = 0 \) in (14).

Two asymptotic behaviour have been found for the p-spin spherical model depending on the choice of the initial conditions [20] [21] [22]:

- True ergodicity breaking: the system equilibrates in a separate ergodic component. Asymptotically time homogeneity and fluctuation-dissipation theorem (FDT) hold [21] [22]. In this case, following [21] [22], we take for the asymptotic form of the two time quantities the Ansatz:

\[
C(t, t') = C_{FDT}(t - t'), \quad R(t, t') = R_{FDT}(t - t')
\]

\[
R_{FDT}(\tau) = -\theta(\tau) \frac{dC_{FDT}(\tau)}{dt}, \quad Q(t, t') = q
\]

\[
\lim_{\tau \to \infty} C_{FDT}(\tau) = q.
\]
• Slow dynamics: the system does not equilibrate. Asymptotically two time sectors can be identified. In the first one (FDT regime), which corresponds to finite time differences \(|t-t'| \sim O(1), \ (t >> 1, \ t' >> 1)|\), the system has a pseudo-equilibrium dynamics since FDT and time translation invariance hold asymptotically. In the second one (ageing regime), which corresponds to “infinite” time differences \(|t-t'| \sim t', \) FDT and time translation invariance do not apply and the system ages \([20]\). In this case, following \([20]\), we take for finite time separations the Ansatz corresponding to equilibrium dynamics, but with \(Q(t',t) = q'\). Whereas for the ageing sector we take the Ansatz \([21]\): 

\[
C(t, t') = q C_{ag}(\lambda), \quad C(t, t') = R_{ag}(\lambda) \tag{17}
\]

\[
R_{ag}(\lambda) = x q \frac{dC}{d\lambda}, \quad Q(t, t') = q' Q_{ag}(\lambda) \tag{18}
\]

\[
C_{ag}(1) = Q_{ag}(1) = 1, \quad \lambda = \frac{t'}{t} \tag{19}
\]

where \(x\) parameterises the violation of FDT \([21]\). 

The asymptotic solutions arising from the previous Ansätze can be grouped in three classes.

1. Equilibrium dynamics.

We denote respectively by \(\lambda^\infty\) and \(m_i^\infty\) the asymptotic values of the spherical multiplier and of the local magnetisations. Plugging the equilibrium dynamics Ansatz into the dynamical TAP equations we find that the equations on \(m_i^\infty\) and \(\lambda^\infty\) are the corresponding static TAP equations. In the asymptotic limit the equations (10) and (11) on the correlation and the response functions reduce to:

\[
\left(\frac{d}{dt} + \lambda^\infty - \mu\right) C(\tau) + \mu + 1 - \lambda^\infty = -\mu \int_0^T d\tau' C(\tau - \tau') p^{-1} \frac{dC(\tau')}{d\tau'} . \tag{20}
\]

The above equation describes the equilibrium dynamics inside the ergodic component associated to a TAP solution \(\{m_i^\infty\}\). Note that this asymptotic dynamical solution is consistent with the assumption of an equilibrium dynamics only if \(\{m_i^\infty\}\) is a local minimum of the free energy.

Since this asymptotic solution represents the equilibration in a stable TAP state \(\{m_i^\infty\}\), it is quite natural to associate to this solution an initial condition belonging to this state. This interpretation is suggested by the results of \([21,22]\). Indeed in \([21,22]\) the low temperature dynamics has been studied starting from an initial condition belonging to the TAP states which are the equilibrium states at a temperature \(T'\). In \([21,22]\) it has been shown that the system relaxes in the TAP states associated to the initial condition. It is easy to show that the equation satisfied by \(C(\tau)\) in \([21,22]\) can be written in the form (20).

Moreover it is interesting to note that the equations (12) on local magnetisations reduce in the long-time limit to a gradient descent in the free energy landscape with an extra term which vanishes at large time.

2. Weak ergodicity breaking.

The asymptotic analysis in the time sector corresponding to finite time differences leads to the same equation (20) for the correlation and the response functions. Whereas for infinite time differences we find that the asymptotic equations admit the solution: \(q' = 0, \ q\) which verifies the equation of the overlap of the threshold states \([22,5,13]\), \(x = (p-2)(1-q)\) and \(C_{ag}(\lambda)\) and \(R_{ag}(\lambda)\), which satisfy the same equations found in \([21]\). The equation (13) on the spherical multiplier reduces to: \(\lambda^\infty = (1-q)^{-1} + \mu(1-q^{p-1})\) and the asymptotic value of the local magnetisations \(m_i^\infty\) is zero. This is exactly the same asymptotic solution found in \([21]\) for random initial conditions. Therefore it is natural to associate to this solution a random initial condition, which is not correlated with any particular stable

\[\text{The asymptotic equations are obtained neglecting the time derivatives. This has as a consequence that from an asymptotic solution we obtain infinitely many others by re-parameterisation [21]. For the sake of clarity in the following we focus on the particular parameterisation shown in equations (17), (18) and (19).}\]
To make a straightforward connection between static free energy landscape and long-time dynamics and to give to the as a gradient descent in the free energy landscape with an extra term going to zero at large time. This result allows one to obtain this asymptotic solution starting from a random initial condition; however for each realization of $h_i(t)$ it is clear that $\lim_{t \to \infty} h_i(t) = 0$ because the equality between $q'$ and $q_h$ is automatically verified in the long-time limit. The vanishing of the local magnetisations is due to the many possible channels that the system can follow in the energy landscape. The role of magnetic fields $h_i(t)$ is to bring the system along one of the possible channel.

3. Between true and weak ergodicity breaking.

In the following we consider the asymptotic solution which corresponds to slow dynamics with $q = q'$. In this case we find the same solution of section II.C.2 except that $q' = q$ and $Q_{ag}(\lambda) = C_{ag}(\lambda)$. As a consequence the local magnetisations do not vanish in the long-time limit. These results indicate that at very large times the system has almost thermalized within a threshold state. Anyway the slow behaviour of the overlap function $Q(t, t')$ implies that the local magnetisations evolve forever, even if more and more slowly. In other words if one waits a time $t_w(>> 1)$ the systems seem to be equilibrated in a certain threshold states on timescales $\Delta t << t_w$; however on timescales of the same order of $t_w$ the system continue to evolve.

To understand the slow evolution of $m_i(t)$ it is important to recall that the threshold states are characterised by a spectrum of the free energy Hessian which is a semicircle law with minimum eigenvalue equal to zero. As a consequence the free energy landscape around threshold states is characterised by almost flat directions. At large times, the equations satisfied by $m_i(t)$ corresponds to a gradient descent in the free energy landscape with an extra term which vanish in the long-time limit. Because of almost flat directions this vanishing term plays a fundamental role and is responsible for ageing. In fact at large times the dynamics takes place only along almost flat directions and this vanishing function of time acts as a vanishing source of drift, so the larger is the time, the weaker is the drift and the slower is the evolution: the system ages.

Finally we remark that it seems natural that the initial conditions related to this asymptotic solution are the configurations typically reached in the long-time dynamics (starting from a random initial condition). In fact a way to obtain this asymptotic solution starting from a random initial condition is to introduce fields $h_i(t)$ which enforce the condition $\lim_{t \to \infty} 1/N \sum_{i=1}^{N} m_i(t)^2 = q' = q_h$ (where $q_h$ is the overlap of threshold states $\{20,28\}$). There are many different way to fix the fields $h_i(t)$ to enforce this condition; however for each realization of $h_i(t)$ it is clear that $\lim_{t \to \infty} h_i(t) = 0$ because the equality between $q'$ and $q_h$ is automatically verified in the long-time limit. The vanishing of the local magnetisations is due to the many possible channels that the system can follow in the energy landscape. The role of magnetic fields $h_i(t)$ is to bring the system along one of the possible channel.

III. FREE ENERGY LANDSCAPE AND LONG-TIME DYNAMICS

At finite times, the dynamics cannot be represented as an evolution in the free energy landscape because the Onsager reaction term in (12) is non-Markovian. However in the long time regime a connection between the free energy landscape and the dynamical evolution can be established.

For initial conditions leading to an equilibrium dynamics, i.e. the equilibration in a stable TAP state $\{m_i^\infty\}$, the equations on the local magnetisations imply that the relaxation of $\{m_i(t)\}$ toward $\{m_i^\infty\}$ coincides with a gradient descent in the free energy landscape with an extra term going to zero at large times. Conversely, in the most interesting and the most physical case of random initial conditions (corresponding to a quench from infinite temperature) the local magnetisations vanish at large times. Anyway a description of the asymptotic dynamics as an evolution in the free energy landscape makes sense also in this case. The local magnetisations vanish asymptotically because the dynamical probability measure at large time tends toward a static probability measure which is broken in separate ergodic components, i.e. the threshold states. One can think at the probability density in configuration space as a wave packet which breaks continuously in sub-packets. Within this picture, the dynamical evolution is characterised by two effects: the cloning of each packet in sub-packets and the slow motion of each single packet. To avoid the spreading of the dynamical measure and to capture only the slow motion, one can take for initial condition a configuration typically reached in the long-time dynamics (starting from random initial conditions). This procedure leads to the asymptotic solution analysed in section II.C.3, in which the correlation and the response functions have the same asymptotic behaviour that for a random initial condition. Moreover $C(t, t')$ and $Q(t, t')$ are equal in the ageing time regime. Thus, also the ageing dynamics obtained starting from a random initial condition can be represented in terms of the equation on $m_i(t)$, i.e. as a motion in the flat directions of the free energy landscape.

In conclusion, through the dynamical TAP approach we have shown that the long-time dynamics can be represented as a gradient descent in the free energy landscape with an extra term going to zero at large time. This result allow one to make a straightforward connection between static free energy landscape and long-time dynamics and to give to the former a meaningful dynamical interpretation. In fact, consider all the stationary and stable dynamical probability...
distributions $P_\alpha(\{s_i(t)\})$. We have shown that the local magnetisations $m^\alpha_i = \langle s_i \rangle_\alpha$ calculated with the probability law $P_\alpha(\{s_i(t)\})$ are the local minima of the TAP free energy. This gives to static TAP solutions a dynamical interpretation in which the properties of stationarity and stability in the free energy landscape are directly related to the properties of stationarity and stability of dynamical distributions $P_\alpha(\{s_i(t)\})$. Moreover the relationship, that we have elucidated, between ageing and flat directions in the free energy landscape allows one to clarify the important role played by the threshold states in the slow dynamics: they are stable states having flat directions in the free energy landscape and as a consequence they are related to ageing dynamics. What is missing to a complete dynamical interpretation of the free energy landscape is the comprehension of the role played by the free energy barriers in the activated dynamics, i.e. to go below the threshold energy starting from random initial conditions. Recent progress in this direction has been done in [24].

IV. CONCLUSIONS

In summary we have found that for the p-spin spherical model the representation of the long-time dynamics as an evolution in the free energy landscape is correct. This evolution consists in a gradient descent in the free energy landscape with an extra term going to zero at large time. This vanishing source of drift depends on the history of the system and is crucial for slow dynamics. Our results explicitly show that the scenario for slow dynamics found at zero temperature [23] remains valid also at finite temperature: ageing is due to the motion in the flat directions of the free energy landscape in presence of a vanishing source of drift. Finally, the relationship between long-time dynamical behaviour and local properties of the free energy landscape, which was already found in [21,22,23], shows up explicitly by the study of the dynamical TAP equations. This relationship is very important not only from a theoretical point of view, but also from a technical one. Indeed it allows to obtain information about the long-time dynamics by a pure static computation [22,23]. For these reasons it would be very interesting to generalise the study performed in this article to finite dimensional systems. In this case the free energy landscape cannot be computed exactly and the long-time dynamics cannot be solved; however, the formal analogies (due to superspace notation) between static and dynamic theory let us hope that one can obtain results on the relationship between long-time dynamics and free energy landscape only using the symmetry properties of the asymptotic solution [23].

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