Barriers in the p-spin interacting spin-glass model. The dynamical approach.

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We investigate the barriers separating metastable states in the spherical p-spin glass model using the instanton method. We show that the problem of finding the barrier heights can be reduced to the causal two-real-replica dynamics. We find the probability for the system to escape one of the highest energy metastable states and the energy barrier corresponding to this process.

One of the most important properties of the spin glasses is the existence of large barriers separating metastable states. The calculation of the barrier heights is not a simple problem even for the long range spin-glass models for which the mean field theory is valid. Although the standard replica approach allows one to find all thermodynamical properties, these properties do not contain information about the barrier heights. The usual dynamical flat approach cannot be used either because it involves taking the limit $N \to \infty$ at an early stage of the calculation, in this limit all barriers become infinite. The modification of the replica approach allowing to estimate the barrier heights was suggested in our previous work Ref. In the present paper we apply this method to the p-spin interacting spin-glass model.

The p-spin interacting model was investigated by the replica, dynamical, and Thouless-Anderson-Palmer (TAP) methods. The qualitative picture arising from these studies is the following. (i) The transition to the spin-glass state is discontinuous. Replica and dynamical theories give different results for the transition temperature, physically the former corresponds to the equilibrium transition and the latter to the dynamical freezing preempting it. (ii) At all temperatures lower than the dynamical transition temperature there is an exponential number of metastable states with energies distributed in some interval $(E_m, E_{CK})$. For a typical state with the energy less than $E_{CK}$ the Hessian of fluctuations has strictly positive eigenvalues so such states are stable, for energies larger than $E_{CK}$ some of these eigenvalues become negative so a typical state is unstable; for energies lower than $E_m$ there are no states. (iii) Dynamical evolution starting from a random configuration leads to a non equilibrium regime exhibiting very slow power law relaxation (aging), in the following we refer to it as Cugliandolo-Kurchan (CK) regime.

The structure of the phase space described above allows one to understand better the physics underlying the aging relaxation found in. The number of states of a given energy, $N_E$, is exponentially large, $S_E = \frac{1}{N} \ln N_E \sim O(1)$ for all energies larger than $E_m$ ($S_{E_m} = 0$); furthermore the complexity, $S_E$, is a monotonic function of the energy, $E$. Thus, a set of all locally stable states is dominated by the states with highest energy, $E_{CK}$, for which these states are still locally stable and dynamics starting from random initial conditions is most likely to end up in one of these most abundant states. A typical state of the largest energy has one eigenvalue which is very close to zero, so the dynamical evolution leads to a marginally stable state but it approaches it very slowly, in agreement with the results of direct dynamical studies. This qualitative argument can be made more precise. At time scales $t$ weakly unstable states with eigenvalues $\lambda < -1/t$ are allowed. Because for the p spin model the maximal energy is directly related to the minimal allowed eigenvalue the states with $\lambda_{\min} \approx -1/t$ dominate the dynamics at time scales $t$. These states are, of course, unstable with the average exponent of the order $\lambda_{\min}$; for the correlation function it means that

$$\partial_t q(t, t') = -\frac{\gamma}{t} q(t, t')$$

with $\gamma \sim 1$. The solution of this equation is a power law relaxation, consistent with the result of the rigorous study. Another conclusion of this reasoning is that the upper bound $E_{CK}$ should be equal to the asymptotic energy of CK regime as, indeed, was found in. Thus, the dynamics starting from random initial conditions (i.e. from a state with $E = 0$) leads to the equilibrium states with $E < E_{CK}$ only in exponentially rare cases. However, as we will show, these equilibrium states can be reached by the dynamical evolution if the system starts from a state with a sufficiently low initial energy, $E < E_c$. This will allow us to study the properties of these states in the framework of the dynamical theory.

Our goal is to find the probability, $P$, for the system to escape one of the highest energy TAP states using the instanton method. Generally, $P \sim \exp N(-E_b/T + S)$ where $E_b$ is the energy barrier corresponding to this transition and $S$ is the entropy (configurational) contribution. Note the important difference with the usual problem of activated transitions, there the contribution from the unique saddle point should be taken into account whereas here the number of saddle points is also exponential which modifies the result. The dependences of the energy barrier $E_b$ and action $A = -E_b/T + S$ on the temperature are plotted in Fig.1. As one expects, the barriers emerge at the dynamical transition temper-
nature. At low temperatures the entropy contribution to the action is negligible and the action is \( A = -E_b/T \).

The idea of our method is the following: Consider the system that is initially in one of the metastable states characterized by the energy \( E_{\text{in}} \), we want to find the probability to escape this state. Let us consider all saddle point trajectories (instantons) leading to transient states with energy \( E_{\text{tr}} > E_{\text{in}} \). Technically we can choose such trajectories inserting an appropriate delta-function constraint in the dynamical functional. After this process the system is left to relax. Apparently, if the transient energy, \( E_{\text{tr}} \), is high enough, the system will relax to the state which is different from the initial one, in this case the spin-spin correlation function \( \langle S(t_i)S(t_f) \rangle \) is zero. On the contrary, if the energy \( E_{\text{tr}} \) is just a little above the energy of the initial stable state \( E_{\text{in}} \), the system will relax to the same state and the spin-spin correlation function \( \langle S(t_i)S(t_f) \rangle \) will be equal to the Edwards-Anderson (EA) order parameter. As we will show, there is a critical value, \( E_c \), of the energy \( E_{\text{tr}} \), such that when \( E_{\text{tr}} < E_c \) the system relaxes back to the same state while for \( E_{\text{tr}} > E_c \) the system escapes. The difference between the critical value of the transient energy \( E_c \) and the energy of the initial stable state \( E_{\text{in}} \) is exactly the barrier energy \( E_b = E_{\text{tr}} - E_{\text{in}} \), and the probability of the instanton transition is determined by the action of the instanton process corresponding to this over barrier.

We now provide the details of the calculation. Using the functional formulation of the dynamical theory (see, for example Ref [14]) we write the spin correlation function as a functional integral

\[
\langle S(t_i)S(t_f) \rangle = \int DS_S(t_i) e^{iS(t_i)^T \mathcal{L}[S(t)]t_i} e^{iS(t_f)^T \mathcal{L}[S(t)]t_f} \delta(\mathcal{H}(t_i) - NE_{\text{tr}}) \delta(\mathcal{H}(t_f) - NE_{\text{tr}}) S(t_i) S(t_f),
\]

where the Lagrangian is

\[
\mathcal{L} = \sum_i -\dot{S}_i^2 - i\dot{S}_i \left( \partial_t S_i + \frac{\delta^2 \mathcal{H}}{\delta S_i^2} \right) + \frac{1}{2} \frac{\delta^2 \mathcal{H}}{\delta S_i^2},
\]

\( \mathcal{H} \) is the Hamiltonian of the p-spin interacting model

\[
\mathcal{H} = -\frac{1}{p!} \sum_{i_1,i_2,...,i_p} J_{i_1,i_2,...,i_p} S_{i_1}S_{i_2}...S_{i_p}.
\]

and \( J_{i_1,i_2,...,i_p} \) is a random symmetric tensor normalized by \( \langle J_{i_1,i_2,...,i_p}^2 \rangle = p!/2N^{p-1} \).

The instanton motion from \( t_i \) to \( t_{tr} \) can be transformed into the usual causal motion with the help of the transformation

\[
S_1(-t) = S(t), \quad i\dot{S}_1(-t) = -\partial_t S(t) + i\dot{S}(t),
\]

where \( t_{tr} = 0 \) was taken to make formulas more compact. In order to distinguish this time interval from the relaxational motion at \( t > t_{tr} \) we denote \( S \) field

\[
S_2(t) = S(t), \quad \dot{S}_2(t) = \dot{S}(t)
\]

for \( t > 0 \). In the new notations the correlation function \( \langle S(t_i)S(t_f) \rangle \) becomes

\[
\langle S(t_i)S(t_f) \rangle = e^{-\beta\Delta\mathcal{E}} \int DS_1 DS_2 e^{i\int_{-t_i}^{t_f} \mathcal{L}[S_1(t)]dt} e^{i\int_{-t_i}^{t_f} \mathcal{L}[S_2(t)]dt} \delta(\mathcal{H}(0) - NE_{\text{tr}})S_1(-t_i)S_2(t_f),
\]

where \( \Delta\mathcal{E} = \mathcal{H}(0) - \mathcal{H}(t_i) \).

We see that Eq. (6) corresponds to the two-real-replica problem with a fixed initial energy. The Green functions become matrices in the replica space

\[
\mathcal{D}_{\alpha,\beta} = \langle S_\alpha S_\beta \rangle, \quad \mathcal{G}_{\alpha,\beta} = \langle S_\alpha i\dot{S}_\beta \rangle, \quad \dot{\mathcal{D}}_{\alpha,\beta} = \langle i\dot{S}_\alpha i\dot{S}_\beta \rangle.
\]

The advantage of this representation is that since Eq. (6) describes the normal (relaxational) motion, the response functions \( \mathcal{G}_{\alpha,\beta} \) are casual and the anomalous Green functions \( \dot{\mathcal{D}}_{\alpha,\beta} \equiv 0 \). Moreover, according to Eq. (6) the replicas are independent from each other, therefore

\[
\mathcal{G}_{1,2}(t_1, t_2) = \mathcal{G}_{2,1}(t_1, t_2) = 0.
\]

Also we will be interested only in the replica-symmetric processes, for which one can write

\[
\mathcal{D}_{1,1}(t_1, t_2) = \mathcal{D}_{2,2}(t_1, t_2) \equiv \mathcal{D}(t_1, t_2),
\]

\[
\mathcal{D}_{1,2}(t_1, t_2) = \mathcal{D}_{2,1}(t_1, t_2) \equiv \mathcal{D}'(t_1, t_2),
\]

\[
\mathcal{G}_{1,1}(t_1, t_2) = \mathcal{G}_{2,2}(t_1, t_2) \equiv \mathcal{G}(t_1, t_2).
\]

Representing the delta-function in (11) as

\[
\delta(\mathcal{H}(0) - NE_{\text{tr}}) = \int d\phi e^{i\phi(\mathcal{H}(0) - NE_{\text{tr}})},\]

we perform averaging over the disorder. Then, making the saddle point approximation we get the equations for the correlation functions:
Green functions depend only on the time difference facts one can integrate Eq.(13) over the limiting value of the energy, can be found analytically: At large times satisfying FDT at large times (the aging form found in Ref.

Thus, we begin with the analysis of the one-replica equations (13,14,16) describe the usual one-replica dynamics, because they do not contain the correlation function $D'$. Therefore, in order to find the most interesting correlation function $D'$ we need first to find $G$ and $D$ solving Eqs.(13,14,16) and then find $D'$ from Eq.(13).

Thus, we begin with the analysis of the one-replica equations (13,14,16). When $E(0) = 0$ the terms emerging from the energy constraint in Eqs.(13,14,16) disappear and the asymptotics of the correlation functions should have the aging form found in Ref. 

where $\gamma$ is a constant depending on temperature. Numerical analysis of Eqs.(13,14,16) shows that this aging regime is still realized when $E(0)$ is higher than some negative critical value $E_c$, which we will find analytically later.

For $E(0) < E_c$ the numerical solution shows that the system relaxes to a stable state with correlation functions satisfying FDT at large times $(t_1, t_2) \gg 1$. In this case the limiting value of the energy, $E_{in}$, and the Edwards-Anderson order parameter, $q$, characterizing this state can be found analytically: At large times $t_1, t_2 \gg 1$ the Green functions depend only on the time difference $t_1 - t_2 = \tau$ and FDT holds $\partial_\tau D(\tau) = -G(\tau)$. Using these facts one can integrate Eq.(13) over $\tau$ obtaining

where $q = D(t + \tau, t), t, \tau \gg 1$. Considering Eq.(14) on times $t_1, t_2 \gg 0$ we get

where $q_1$ is the overlap between the initial and final states $q_1 = D(t, 0), t \gg 1$. The equation closing the system follows form Eq.(16)

Combining Eqs.(13,14,16) and introducing a new variable $z = \beta(1 - q)$ $q(\beta/2)$ we get the equation

which contains only one parameter $E_{tr}$. Therefore, all the temperature dependence of $q$ (at fixed $E_{tr}$) comes from the equation $z = \beta(1 - q)$ $q(\beta/2)$, this agrees with TAP approach of Ref. One can show that Eq.(20) has solutions only when $E_{tr} < E_c$, with

which is related to the dynamical transition temperature $T_c$ by $E_c = -1/2T_c$. For $E_{tr} < E_c$ Eq.(20) has two solutions but only one of these solutions is physical, it lies in the interval $0 < z < z_c$ with $z_c = \sqrt{2/(p-1)}$.

Eqs.(17,18,19) can be solved analytically for one special value of the energy $E = -\beta/2$. In this case $E = E_{tr}, q = q$ and Eqs.(17,18,19) are reduced to a single equation

This special value of the energy has a simple physical meaning: The system remains at the same state and it is at equilibrium at all times during the process.

To summarize the results of one-replica dynamics: When $E_{tr} > E_c$ the system relaxes to the aging CK state, when $E_{tr} < E_c$ the system relaxes to one of the locally stable states. There is a special value $E_{tr} = -\beta/2$ such that the system is at the equilibrium for all times.

Now turn to the behavior of the correlation function $D'$. Numerical solution of Eq.(13) gives the following asymptotics of the correlation function $D'$:

$$E_{tr} < E_c : \quad D'(t_1, t_2) \to q_{EA}, \quad t_1, t_2 \to \infty,$$

$$E_{tr} > E_c : \quad D'(t_1, t_2) \to 0, \quad t_1, t_2 \to \infty.$$  

It means that for energies $E_{tr} < E_c$ the replicas relax to the same state, while for $E_{tr} > E_c$ to different ones. For the original problem it means that when $E_{tr} < E_c$ the system remains in the same TAP state after the instanton process, while for $E_{tr} > E_c$ the system escapes the original state. The result (24) can also be obtained analytically by considering Eq.(13) and assuming that FDT holds at large times. Thus we conclude that $E_b = E_c - E_{in}$ is the energy of the barriers between the
highest energy TAP states. The height of the barrier $E_b$ as a function of temperature is plotted on Fig.1.

The probability to escape a metastable state is $e^{NA}$ where the action $A$ is

$$A = \frac{1}{N} \ln \int DS \ e^{\int_0^\beta L(S)}. \quad (25)$$

The differentiation of (25) with respect to $\beta$ gives

$$\frac{dA}{d\beta} = -\frac{1}{N(p-1)!} \int_{t_1}^{t_{\text{inst}}} \langle \sum J_{1,2,\ldots ip} iS_1 S_2 \cdots S_{ip} \rangle_{S,J}.$$ 

Using the transformation law (4,5) we get

$$\frac{dA}{d\beta} = -\frac{\mathcal{H}(0) + \mathcal{H}(t_1)}{N} = -E_{\text{tr}} + E_{in}. \quad (26)$$

To integrate (26) it is convenient to use the result for the free energy of TAP states of Ref. 2

$$f_{in} = -q^{\frac{7}{2}} \left( \frac{1}{pz} + \frac{1}{2}z(p-1) \right) - \frac{T}{2} \ln(1 - q) - \frac{\beta}{4} (1 + (p-1)q^p - pq^{p-1}). \quad (27)$$

Note that this expression does not contain the complexity contribution. Using Eqs. (20,27) one can check that

$$E_{in} = \frac{d}{d\beta} \beta f_{in}. \quad (28)$$

Therefore for the action we have

$$A = \beta f_{in} - E_{tr} \beta - \Gamma(E_{tr}), \quad (29)$$

where $\Gamma$ is an unknown function which depends only on $E_{tr}$. This function can be found from the following arguments. As was shown above there is a special value of $E_{tr} = -\beta/2$ for which the system is at equilibrium for all times. It means that actually there is no instanton motion, therefore the action of this process is zero. Imposing this requirement and using Eq. (22) we find $\Gamma$, inserting it in (29) we finally get

$$-A = E_{tr}^2 + E_{tr} \beta - [\beta f_{in} - g(z)], \quad (30)$$

where

$$g(z) = \frac{1}{2} \left( \frac{2-p}{p} - \ln \frac{p - 1}{2} - \frac{z^2 - 2}{p^2 z^2} \right), \quad (31)$$

and $z$ is determined by Eq. (20). The function $g(z)$ turns out to be the same as the complexity of the free energy minima found in Ref. 3.

In order to get the action which determines the probability to escape a metastable state one should take $E_{tr} = E_c$ in (30). The result is plotted in Fig.1.

The result (30) can be presented in a very simple form if we introduce the "full" free energy including complexity following Ref. 5

$$\tilde{f}(T) = f_{in} - Tg - T(1 + \ln(2\pi))/2, \quad (32)$$

where the third term corresponds to the conventional normalization of the trace over spins. We define the 'free energy' of a random state $f_{R}$ with a given energy $E$ as

$$f_{R}(E) = E - T S_{R}, \quad (33)$$

where $S_R$ is the 'entropy' of the random state defined by

$$\langle \delta(N E - \mathcal{H}(S)) \rangle_f = e^{N S_R}. \quad (34)$$

The straightforward calculation gives $S_R(E) = (\ln 2\pi + 1)/2 - E^2$. Then the action $A$ becomes

$$-A = [f_R(E_{tr}, T) - \tilde{f}(T)]/T. \quad (35)$$

We see that with these definitions of the free energies the action has a form corresponding to the Gibbs rule.

In conclusion, we found the energy barriers between metastable states with energies $E \approx E_{CK}$. $E < E_{CK}$ using the instanton method. Mapping of the instanton motion into the usual motion going back in time allows to reduce the problem to the causal two-real-replica dynamics. The probability to escape a metastable state is determined by the action of the instanton process, this action is expressed through the "full" free energy of the system that includes complexity. The method developed in the paper can be applied to study the free energy structure of other spin-glasses. The drawback of this method is that it does not allow one to find all saddle point trajectories, instead it finds only a typical one, corresponding to a typical barrier; in particular, in the p-spin model we were able to study only the transitions between the most abundant states with $E \approx E_{CK}$. Ideally one wants to know the barrier (or distribution of barriers) separating two states with given energies; this is a much more difficult problem which remains unresolved.

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1. M. Mezard, G. Parisi and M. A. Virasoro, *Spin Glasses and Beyond* (World Scientific, 1987)
2. A. Cavagna, I. Giardina and G. Parisi, cond-mat/9702060
3. A.V. Lopatin and L.B. Ioffe, cond-mat/9904211
4. A. Crisanti and H.-J. Sommers, Z. Phys. B 87, 341 (1992)
5. A. Crisanti, H. Horner and H.-J. Sommers, Z. Phys. B 92, 257 (1993)
6. L.F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. B 71, 173 (1993)
7. A. Crisanti and H.-J. Sommers, J. Phys. I France 5, 805 (1995)
8. K.H. Fischer and J.A. Hertz, *Spin Glasses* (Cambridge University Press, 1993)