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LETTER TO THE EDITOR

Replica-symmetry breaking in long-range glass models without quenched disorder

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Abstract

We discuss mean-field theory of glasses without quenched disorder focusing on the justification of the replica approach to thermodynamics. We emphasize the assumptions implicit in this method and discuss how they can be verified. The formalism is applied to the long-range Ising model with an orthogonal coupling matrix. We find the one-step replica-symmetry-breaking solution and show that it is stable in the intermediate-temperature range that includes the glass state but excludes very low temperatures. At very low temperatures this solution becomes unstable and this approach fails.

The thermodynamics of glasses without quenched disorder is a long-standing problem in statistical physics. The interest in this problem was renewed recently when it was understood that powerful methods developed for the glasses with quenched disorder can often be applied to this problem [1–6]. In both systems the local magnetization (or local density in the case of structural glasses) in the ground state varies from site to site and different sites are typically non-equivalent. The qualitative reason for glasses without quenched disorder being more difficult to describe theoretically than spin glasses is the following. The mean-field theory has to operate with the average magnetization (or its moments), not with quantities which depend on a realization and a particular state. The average quantities appear naturally in spin glasses after averaging over quenched disorder which makes all sites equivalent.

A few methods were suggested to overcome this difficulty for the glasses without quenched disorder. First, a mapping of some glass models to the quenched disordered problems was suggested [1]; this method has the obvious disadvantage that such a mapping is difficult to guess. Second, it was noted that a typical dynamics in a glassy system leads not to a ground state but to one of many metastable states, providing an effective averaging mechanism [7] which makes all sites equivalent even for glasses without quenched disorder. This method has the disadvantage that dynamical equations are much more difficult to solve than statical ones. Very recently the cloning method was proposed that is based on the idea that even at low T a system of m clones might be distributed in its phase space over many low-lying metastable states if m is chosen correctly and the properties of all these states are essentially equivalent to those of the ground state [3–6]. Generally, the partition sum of m weakly coupled clones is $\sum_F \mathrm{e}^{-N(m\beta F - S_{conf}(F))}$, where the sum is over free energies (per site) of metastable states,

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F, and $S_{conf}(F)$ is their configurational entropy ($S_{conf} = (1/N)\ln(\mathcal{N}_{states})$). Assuming that $\mathrm{d}S_{conf}(F)/\mathrm{d}F$ is finite at the lowest F associated with the ground state, one needs to chose $m \propto T$ at low T in order to avoid a complete dominance by a single (ground) state and the problems with site non-equivalence mentioned above. Distributing the system in the phase space provides the effective averaging mechanism in this approach. The main assumptions implicit in this approach are that low-lying metastable states are not correlated (otherwise, averaging over them would not remove completely the non-equivalence of different sites) and that configurational entropy associated with these states behaves well as a function of energy at low energies permitting the 'right' choice of m.

The goal of this letter is to provide a theoretical framework alternative to the cloning method which, albeit somewhat similar in formalism, uses different physical arguments for its justification and allows one to check the main assumption of the method mentioned above. The main idea of the approach is that in a system with many low-lying states, even a small random field is able to change the energy balance between the states and pull down a different state making it a new ground state of the system. Averaging over this random field is equivalent to the averaging over low-lying metastable states. Specifically, in a spin system we add to the physical Hamiltonian a magnetic field part: $\mathcal{H} \to \mathcal{H} + \sum_i h_i S_i$ with small random h_i, negligible in the thermodynamic limit. The resulting change in the energy of a typical metastable state is of the order of $\sqrt{N}h$; because this energy interval contains a large amount of metastable states, we expect that a small non-zero field would result in a large rearrangement of their energies but would not change the properties of individual states. Averaging over the random field configurations is performed in the usual way introducing n replicas of the system and taking the limit $n \to 0$. The assumption of uncorrelated states is equivalent to one-step replica-symmetry-breaking (1RSB) formalism; in this case only replicas belonging to the same block are correlated and the replica method becomes equivalent to the cloned liquid approach with the number of clones being equivalent to the size of the 1RSB block [6]. From the above discussion it is evident that another assumption implicit in this approach is that the energy spacing between low-lying states should be much less than $\mathrm{O}(\sqrt{N})$; if it is too big, a small magnetic field will not be sufficient to rearrange low-lying states, while if it is too small, e.g. $\mathrm{d}S_{conf}/\mathrm{d}F|_{F_0} = \infty$, the effect of the random field will be too large and no sensible limit $h_i \to 0$ is possible. The latter situation seems to happen in the periodic long-range Josephson array with flux 2π per strip [2] when all states are exactly degenerate and $S_{conf}(F)$ is very singular at $T = 0$.

We apply our method to the Ising version of the periodic long-range Josephson array model which is a simple example of a glass without quenched disorder and we show that in this model the main assumptions of the method are correct in the intermediate-temperature range but become wrong at very low temperatures. That is, we show that the 1RSB solution that we find is stable in the intermediate range of temperatures, but becomes unstable at very low temperatures.

The generic physical properties of the 1RSB solution are best illustrated by the p-spin model which was extensively studied by various methods and for which the 1RSB *ansatz* gives an exact solution at all temperatures. In this model one identifies two distinct transition temperatures—the dynamical one, T_g, at which the metastable states first appear, and the static one, T_c, corresponding to an equilibrium thermodynamic phase transition [8–10]. The configuration entropy associated with metastable states of a particular energy is a monotonically increasing function of the energy (at fixed temperature) [11], so the states with largest possible energy dominate the full configurational entropy. Furthermore, a typical volume of the attraction basins of each state is only a weak function of the energy, so a typical dynamical process starting with random initial conditions ends up in one of the most abundant states, i.e. a

state with the highest energy. Low-lying metastable states can be reached only by very special dynamical processes that start with special initial conditions, such as constraint on initial energy [12]. In contrast to the dynamics, the thermodynamics involves averaging with Gibbs weight and, thus, probes mostly the lowest-lying metastable states; the configurational entropy of these states is negligible. Generally, one expects replica theory to imply thermodynamical averaging and to probe only the lowest energy states. Few approaches have been invented to probe states with higher energies within the replica formalism. The situation is simplest in the case of the 1RSB *ansatz*; here one replaces the condition that the free energy is minimal as a function of the *ansatz* parameter, m, by the condition that resulting states are marginally stable. We use this procedure in our approach to determine both the thermodynamic transition temperature (as the clone method does) and the dynamical one.

We now provide the details of our formalism and its application to the simplest mean-field model of a glass without disorder. Our model consists of two sets of Ising spins (which we shall refer to as 'upper' and 'lower' in the following) interacting via

$$\mathcal{H} = -\frac{1}{2}\sum_{m,n} S_{im} J_{mn}^{ij} S_{jn}. \tag{1}$$

Here the spin S_{im} has a site index ($m = 1, \ldots, N$) and a component index $i = 1, 2$ corresponding to the upper and lower spins, and matrix $\hat{J}$ is

$$\hat{J}_{mn} = \begin{pmatrix} 0 & J_{mn} \\ J_{mn} & 0 \end{pmatrix} \tag{2}$$

with

$$J_{mn} = (J_0\sqrt{2/N}) \cos\left(\frac{2\pi\alpha}{N}(m - 1/2)(n - 1/2)\right).$$

For $\alpha = 1/2$ we obtain the orthogonal limit

$$\sum_n J_{mn} J_{nk} = J_0^2 \delta_{mk}.$$

In what follows we shall focus on this case. This Ising spin model is similar to the XY spin model of the long-ranged Josephson array [2] and to the Bernasconi model [13]. Like in these models, its lowest states correspond to 'pseudorandom' sequences with flat Fourier transform. So, we expect this model to also display glassy properties—in particular, that it has extensive configurational entropy at low temperatures. Further, one expects that in a model with long-range interaction the barriers separating metastable states become infinite in the thermodynamic limit. We have verified numerically that the configurational entropy in this model is indeed extensive and its dependence on energy is similar to the one obtained for other infinite-range glasses (see figure 1). Note, however, the important difference between this model and the XY spin model of [2]: in the orthogonal limit the ground state of the Ising model does not become extensively degenerate (see figure 1), whereas in the XY spin model the ground state becomes extensively degenerate in the unitary limit making it very complicated [2].

Taking the Gaussian distribution for the random magnetic field $\langle h_i h_j \rangle = 2h_0^2 \delta_{i,j}$ we get the replica Hamiltonian

$$\mathcal{H}_s = \sum_\alpha \mathcal{H}(S_\alpha) + h_0^2 \sum_{\alpha,\beta,i} S_{im}^\alpha S_{im}^\beta \tag{3}$$

where the replica indices α, β run from 1 to n and the limit $n \to 0$ should be taken. The glass transition corresponds to the appearance of a non-replica-symmetric solution of the saddle-point equations associated with Hamiltonian (3) in the limit $h_0 \to 0$.

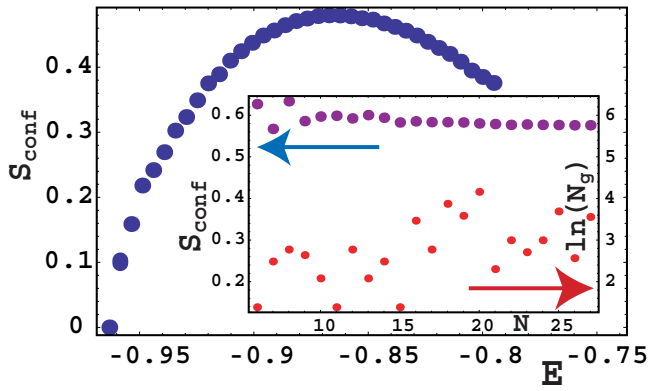

Figure 1. Main panel: configurational entropy $S_{conf} = \ln(\mathcal{N})/N$ at $T = 0$ as a function of state energy obtained from direct numerical simulations on systems up to $N = 27$ size. Inset: the total S_{conf} and the degeneracy, N_g, of the lowest energy state at $T = 0$ as a function of system size.

In the large-N limit a long-range model containing N sites can be reduced to an effective single-site model with a free-energy density $\mathcal{F}$:

$$-\beta\mathcal{F} = \frac{1}{2}\operatorname{Tr}\gamma(B) + \frac{1}{2}\sum_j S_j^\alpha B_{\alpha\beta} S_j^\beta \tag{4}$$

where S_j^α is an Ising spin field retaining only replica and component index dependence, B is an order parameter matrix in the replica space. The function $\gamma(B)$ can be determined from the condition that all single-site correlation functions of the model (4) coincide with the correlation functions of the original model (3). Instead of comparing the spin correlation functions of these two models it is easier to decouple Ising spins using the auxiliary field ψ, sum over Ising spins and compare the correlation functions of the conjugate field ψ in the two new models:

$$\beta\mathcal{H}_\psi = \frac{T}{2}\sum_{m,n,\alpha}\psi_{im}^\alpha(\hat{J}^{-1})_{mn}^{ij}\psi_{jn}^\alpha - \sum_{m,\alpha,j}V(\psi_{jm}^\alpha) \tag{5}$$

$$\beta\mathcal{F}_\psi = -\frac{1}{2}\left[\operatorname{Tr}\gamma(B) - \sum_{\alpha,\beta,j}\psi_j^\alpha B_{\alpha\beta}^{-1}\psi_j^\beta\right] - \sum_{\alpha,j}V(\psi_j^\alpha) \tag{6}$$

where $V(\psi) = \ln 2\cosh(\psi)$. For both models one can construct a formal perturbation theory in the interaction $\ln 2\cosh(\psi_\alpha^{(j)})$ and verify that these expansions coincide. We begin with the model (5). Inspecting the terms of the perturbation theory for the correlator

$$G_{im,jn}^{\alpha\beta} = \langle\psi_{im}^\alpha\psi_{jn}^\beta\rangle$$

one verifies that in the leading order in $1/N$ it is given by $\hat{G} = [T\hat{J}^{-1} - \Sigma]^{-1}$ with the self-energy Σ which is diagonal in the site index: $\Sigma = \mathcal{A}\delta_{mn}\delta_{i,j}$. This approach is similar to a locator expansion [14] but in our case the locator $\mathcal{A}$ might be non-trivial in the replica space. Using the orthogonality of $\hat{J}$ we obtain that the single-site correlation function $\mathcal{G}_{\alpha\beta} \equiv G_{im,im}^{\alpha\beta}$ (which we need to establish the correspondence between the models) becomes

$$\mathcal{G} = [-\mathcal{A} + (j_0^2\mathcal{A})^{-1}]^{-1} \tag{7}$$

where $j_0 = \beta J$.

Now we turn to the model (6). Here the self-energy is diagonal in the site index by construction; further, the interaction part of this model is the same as for model (5); assuming

that their single-site correlation functions coincide, we conclude that their single-site self-energies are equal as well. Thus, the spin correlator obtained for this model is $\mathcal{G} = [B^{-1} - \mathcal{A}]^{-1}$; comparing this expression with (7), we conclude that $B = j_0^2 \mathcal{A}$.

The correlator of the dual field ψ can be related to the correlator of original spins: consider a Gaussian transformation leading to the model (6):

$$\exp(SBS/2) = \int \mathrm{d}\psi \ \exp(-\psi B^{-1}\psi/2 + S\psi)$$

and use it to express $\mathcal{G}$ via the correlator $D_{\alpha\beta} \equiv \langle S^\alpha S^\beta \rangle$; we get: $\mathcal{G} = B + BDB$. Solving this equation for the spin correlator D and using (7) and the relation $B = j_0^2 \mathcal{A}$ we obtain

$$D = B[j_0^2 - B^2]^{-1}. \tag{8}$$

Finally, the saddle-point condition for the free energy (4) is $2D = -\gamma'(B)$; therefore integrating equation (8) we find

$$\gamma(B) = \ln(1 - j_0^{-2} B^2). \tag{9}$$

Note that the free energy (4) coincides with the free energy of the model considered in reference [1] although their properties at finite N are markedly different. Furthermore, this free energy is the same as that obtained by the fiduciary Hamiltonian approach [1].

Paramagnetic state. In this state we take the replica-symmetric *ansatz* $B_{\alpha,\beta} = \mu \delta_{\alpha,\beta}$ and the free energy (4) becomes

$$\mathcal{F}/T = [\ln j_0^2 - \ln(j_0^2 - \mu^2)]/2 - \mu - 2\ln 2. \tag{10}$$

Variation with respect to μ gives

$$\mu = [\pm\sqrt{1 + 4j_0^2} - 1]/2.$$

Here we take the upper sign because another solution leads to an unphysical positive answer for the energy. Usual thermodynamic relations between energy and entropy give $E = -T\mu$, $S = \ln[4\sqrt{\mu}/j_0]$.

One can see that the entropy of the normal solution becomes negative at $T < T_{S=0} = J_0/(4\sqrt{15}) \approx 0.064\,550\, J_0$. The fact that the entropy of a supercooled liquid (normalized to a corresponding crystal state) interpolated to low temperatures becomes negative at some non-zero temperature was first observed by Kauzmann [15]. Thus one expects the thermodynamic glass transition to take place at some temperature, T_c, above $T_{S=0}$.

Glass state. At the thermodynamic glass transition temperature T_c the replica symmetry is broken; we assume that it is described by 1RSB and then verify that it is indeed a stable solution below T_c. The 1RSB *ansatz* is $B_{\alpha,\beta} = \mu\delta_{\alpha,\beta} + \eta R_{\alpha,\beta}$, where the matrix R is a block-diagonal matrix consisting of $m \times m$ blocks with all elements equal to 1; we get the free-energy functional

$$\beta\mathcal{F} = [\log j_0^2 - (1 - 1/m)\ln(j_0^2 - \mu^2)]/2 - 2\ln 2 - (\ln X)/2m - \mu - 2f(\eta, m)/m \tag{11}$$

where $X = j_0^2 - (\mu + \eta m)^2$ and the function f is

$$f(\eta, m) = \ln\left[\int P_m(z)\, \mathrm{d}z\right] \qquad P_m(z) = \frac{\mathrm{e}^{-z^2/2}}{\sqrt{2\pi}} \cosh^m(z\sqrt{\eta}). \tag{12}$$

Taking the derivatives of $\mathcal{F}$ with respect to μ, η, m, we get

$$\left(\frac{1}{m} - 1\right)\frac{\mu}{j_0^2 - \mu^2} - \frac{\eta m + \mu}{Xm} + 1 = 0 \tag{13}$$

$$-(\eta m + \mu)/X + q(m - 1) + 1 = 0 \tag{14}$$

$$\frac{1}{2m^2}\log\left[(j_0^2 - \mu^2)/X\right] + \frac{2}{m}\frac{\partial}{\partial m} f(\eta, m) - \eta(\mu + \eta m)/mX - 2f(\eta, m)/m^2 = 0 \tag{15}$$

where

$$q = \int \tanh^2(z) P_m(z)\, \mathrm{d}z \Big/ \int P_m(z)\, \mathrm{d}z$$

is the spin overlap of different replicas belonging to the same block $D_{\alpha,\beta} = (1-q)\delta_{\alpha,\beta} + qR_{\alpha,\beta}$, which coincides with the Edwards–Anderson (EA) order parameter. Equations (13), (14) can be solved with respect to m, η giving

$$\mu = \eta \frac{1 + (1 - q + qm)\eta m}{q/(1-q) - 2\eta(1 - q + qm)} \tag{16}$$

and $j_0^2 = \mu^2 + \mu/(1-q)$. For a given m we can solve equation (15) numerically with respect to η and get all quantities as functions of m. The resulting dependence of $m(T)$ for $J_0 = 1$ is shown in figure 2. In the limit $n \to 0$, the values of m should lie within the interval (0, 1) and $m = 1$ defines the thermodynamic critical temperature $T_c \approx 0.064\,593$; it is larger than $T_{S=0}$ as expected. The value of the EA order parameter q at the thermodynamic glass transition is very close to 1, $1-q = 0.000\,171\,16$, so in this sense the phase transition is strongly first order but (similarly to in the p-spin model) the energy and entropy do not change discontinuously at the transition. The numerical solution shows that when the temperature decreases, the entropy of the glass state monotonically decreases and eventually becomes negative below $T' \approx 2.8 \times 10^{-4}$. The explanation of such unphysical behaviour is that the 1RSB *ansatz*, in fact, becomes unstable in this low-temperature regime.

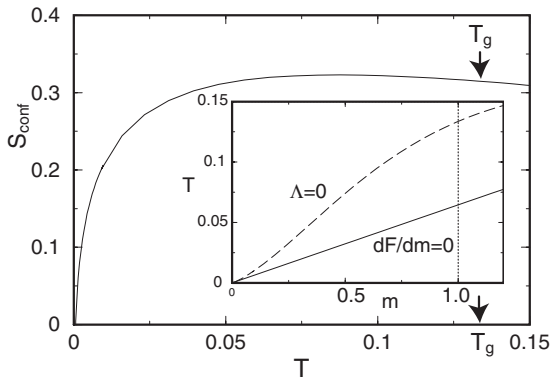

Figure 2. Main plot: the dependence of the configuration entropy on the temperature for the marginally stable solution. Inset: the size of the 1RSB block, m, for thermodynamic (solid line) and marginally stable (dashed line) solutions. The value of T at which $m = 1$ gives the thermodynamical (dynamical) critical temperature.

Stability of the thermodynamical solution. In order to analyse the stability of the 1RSB *ansatz* we expand equation (4) to second order in the fluctuation of the order parameter δB and consider different families of fluctuation matrices δB. This calculation is very similar to the analysis of the stability of the paramagnetic solution and the Parisi solution in the SK model [16, 17], so we only sketch it here[1]. We find that the most dangerous direction in the fluctuation space corresponds to the 'replicon' modes [16, 17] which are fluctuations within diagonal blocks of δB satisfying the conditions $(\delta B\, R)_{\alpha,\beta} = 0$, $\delta B_{\alpha,\alpha} = 0$. The eigenvalue corresponding to these modes is

$$\Lambda = 2(1-q)/\mu + 2(1-q)^2 - 2(r - q^2)$$

[1] The details of this analysis will be presented elsewhere.

where

$$r = \int \tanh^4(z) P_m(z)\, \mathrm{d}z \Big/ \int P_m(z)\, \mathrm{d}z.$$

Numerical solution shows that Λ is positive at temperatures $T > T_{uns} \approx 6.1 \times 10^{-3}$ but changes sign at T_{uns}; thus the 1RSB solution is unstable at $T < T_{uns}$.

Marginal solution. One expects that in a glass a typical dynamical process will lead to a most abundant state which is, therefore, marginally stable. We note that, although plausible, this assumption might be violated if the attraction basins of the low-lying states are much larger than those of the marginally stable ones [18]. Assuming that it is not the case, a dynamical freezing leads to the states with $\Lambda = 0$ instead of the states with the minimal free energy characterized by $\partial\mathcal{F}/\partial m = 0$. Thus, to get the properties of the states selected in a 'dynamical' process, we replace equation (15) by $\Lambda = 0$. The resulting dependence of the temperature on the size of the 1RSB block m is shown in figure 2. The value $m = 1$ defines the 'dynamical' critical temperature $T_g \approx 0.133\,63$. The free-energy functional (4) corresponding to the 1RSB *ansatz* is equivalent to the free-energy functional that is obtained in the cloned liquid approach with m being equal to the number of clones [6]. The stability of the 1RSB solution indicates that the main assumptions of this approach are correct in some temperature range below T_g and, therefore, in this temperature range the configurational entropy is given by $S_{conf} = m^2\, \partial\mathcal{F}/\partial m$. The dependence of S_{conf} corresponding to the marginal solution on temperature is shown in figure 2. Decreasing the temperature, it first increases, goes through the maximum at T_m, and eventually becomes negative at the temperature T_{uns}, at which the thermodynamical solution becomes unstable. It is not clear however that the 1RSB solution is a correct solution over the whole temperature range $T_{uns} < T < T_g$; on the contrary, it is quite likely that another solution is preferred by the system below some $T_c' < T_g$. We have only indirect arguments for this: first, it seems unphysical that S_{conf} decreases with temperature decrease: in the SK model the total configuration entropy of metastable states increases with temperature decrease (corresponding to the appearance of new states at lower T), while in the p-spin model the configuration entropy does not depend on temperature at all; second, the S_{conf} obtained does not match the results of the numerical simulations if one believes that this solution remains correct at $T < T_m$. Finally, note the analogy with higher temperatures: the paramagnetic solution is always stable but is eventually replaced by the 1RSB solution.

In conclusion, we have justified the application of the replica method to some systems without quenched disorder and discussed situations in which it fails. We identify two dangers: correlations between metastable states close to the ground state and too-large degeneracy of the ground state. We apply the formalism to the periodic Ising spin model with an orthogonal coupling matrix and find that it gives the same free energy as the fiduciary Hamiltonian approach [1]. Further, we show that it works in the intermediate-temperature range but fails at low temperatures when metastable states become correlated. Two questions remain open: whether the generalization of this method to continuous symmetry breaking would allow one to study the models with correlated metastable states and what to do if the ground state of the model is highly degenerate as it is, e.g., in the case of a unitary coupling matrix.

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