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LETTER TO THE EDITOR

Metastable states in the Blume–Emery–Griffiths spin-glass model

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Abstract

We study the Blume-Emery-Griffiths spin-glass model in the presence of an attractive coupling between real replicas, and evaluate the effective potential as a function of the density overlap. We find that there is a region, above the first-order transition of the model, where metastable states with a large density overlap exist. The line where these metastable states appear should correspond to a purely dynamical transition, with a breaking of ergodicity. Differently from what happens in p-spin glasses, in this model the dynamical transition would not be the precursor of a one-step replica symmetry breaking transition, but (probably) of a full replica symmetry breaking transition.

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The Blume–Emery–Griffiths (BEG) spin-glass model [1, 2] can be seen as a generalization of the Sherrington–Kirkpatrick (SK) model, in which each site carries, in addition to the spin variable $S_i = \pm 1$, a lattice gas variable $n_i = 0, 1$. Its Hamiltonian is given by

$$\mathcal{H} = -\sum_{i<j} J_{ij} S_i S_j n_i n_j - \frac{K}{N} \sum_{i<j} n_i n_j - \mu \sum_i n_i \tag{1}$$

where J_{ij} are quenched Gaussian variables with zero mean and variance J^2/N. The case $K/J = 0$ is also known as the Ghatak–Sherrington model [3]. It has been found that, in general, for a fixed value K/J, there exists a tricritical point in the phase space. For higher temperature or chemical potential the model presents a second-order transition from a paramagnetic to a spin-glass phase. For lower temperature or chemical potential, the transition becomes first order, with a jump in the mean density $d = \langle n_i \rangle$ and overlap $q_{\alpha\beta} = \langle S_i^\alpha n_i^\alpha S_i^\beta n_i^\beta \rangle$ between two replicas α and β (see figure 1 for the case $K/J = 0$). Although the overlap parameter can become discontinuous, the transition seems to be quite different from the transition of other discontinuous spin glasses, such as the p-spin models. A first obvious difference is that the transition of the BEG spin glass is first order also in the Ehrenfest sense, i.e. with a jump in the

mean energy and entropy. Moreover, while in p-spin models the first step of replica symmetry breaking (RSB) turns out to be exact, in the BEG spin glass the question of the order of RSB appears much more subtle. The question was studied by many authors in the case of the Ghatak–Sherrington model [4–6]. It was found that the replica symmetric solution is unstable against RSB in the whole spin-glass region, with the appearance of complex eigenvalues in the stability matrix. Recently [7], it has been shown that this kind of instability persists also in the one-step RSB solution. Therefore it seems reasonable that only a full RSB may probably give the correct solution, as happens in the SK model.

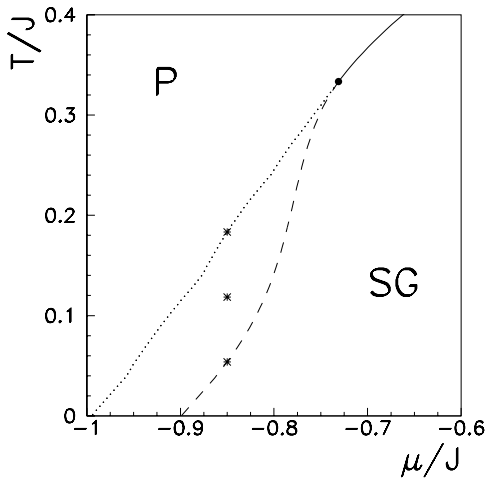

Figure 1. Phase diagram of the model for $K/J = 0$. The region P is the paramagnetic phase, while the region SG is the spin-glass phase. The full curve is the line of second-order transitions, terminating at the tricritical point (black dot). The dashed curve is the line of first-order transitions, and the dotted one is the line where non-paramagnetic solutions of the saddle point equations first appear. The three asterisks are the points where we have calculated the effective potential (see figure 2).

In recent years, a version of the model called frustrated Ising lattice gas (FILG), has been extensively studied as a model of a structural glass [8–15]. In this version the disordered interactions are of the type $J_{ij} = \pm J$, and $K = -J$. Indeed, the FILG can be interpreted as a model for a system of asymmetrical molecules, with the variables n_i representing the presence of a molecule on the site i, and the variables S_i representing the spatial orientation of the molecule. Two neighbouring particles feel a repulsion of intensity $2J$ if their relative orientation is 'wrong', i.e. if $J_{ij}S_iS_j < 0$. Numerical simulations on finite-dimensional lattices show that at low temperature the model develops a two-step relaxation [8–11], as observed in supercooled liquids and predicted by the mode coupling theory (MCT) of the glass transition [16].

Given these links between the model and the glass transition in structural liquids, it would be interesting to study (at least in mean field) if the discontinuous transition of the model is preceded at a higher temperature by a purely dynamical transition, from an ergodic to a non-ergodic phase, as it happens for p-spin glasses [17, 18]. This would require the solution of the dynamical equations, as done for the p-spin, to see if they show a singularity, and of what kind, at some temperature greater than the static one. In this letter we address the problem from another point of view, exploiting the effective potential theory, introduced some time ago [19–22] as a tool to identify the presence of metastable states, and a transition from an

ergodic to a non-ergodic phase. We will refer to the so-called 'annealed version' of the method. One considers two 'real' replicas of the system (as opposed to the replicas generated by the replica trick), labelled 1 and 2, and defines a 'degree of similarity', i.e. an overlap q, between them. Then one studies the system composed by the coupled replicas, with Hamiltonian $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 - \epsilon q$. If $F(\epsilon)$ is the free energy of the coupled system, then the Legendre transform $V(q) = \max_{\epsilon}[F(\epsilon) + \epsilon q]$ will represent the 'effective potential' as a function of the overlap q, i.e. the work needed to keep the two replicas, in the configuration space, at the distance q. What one finds in p-spin models [19–21] and in structural glasses in the hypernetted chain approximation [23, 24], and expects generally whenever metastable states are present in the system (i.e. for temperatures between the static and dynamical transition) is that the potential $V(q)$ presents two minima. A lower minimum, for low values of the overlap q, corresponds to the 'unbounded state', in which the two replicas are in different 'valleys' of the configuration space. A second higher minimum, for high values of q, corresponds to the 'bounded state', in which the two replicas are constrained to stay in the same valley. As the free energy of each single system is independent from which valley the system is in, the gap ΔV between the two minima can be interpreted as being equal to $T\Sigma$, where Σ is the logarithm of the number of valleys, and is called complexity or configurational entropy.

We apply the effective potential theory to the model defined by (1) with $K/J = 0$. The phase space is depicted in figure 1, where the continuous curve represents the line of second-order transition, the black dot the tricritical point, and the dashed curve the line of first-order transitions. We now introduce two real replicas, coupled in the density overlap $q_d = \frac{1}{N}\sum_i n_i^1 n_i^2$. The Hamiltonian of the system is

$$\mathcal{H} = -\sum_{a=1,2}\left(\sum_{i<j} J_{ij} S_i^a S_j^a n_i^a n_j^a + \mu \sum_i n_i^a\right) - \epsilon \sum_i n_i^1 n_i^2 \tag{2}$$

where $a = 1, 2$ is the label of the real replica. By the usual replica trick, we can write the free energy of the system as

$$F = \frac{\beta J^2}{2}(d^2 + q_s^2) + \frac{\beta J^2}{n}\sum_{\alpha<\beta}(q_{\alpha\beta}^2 + p_{\alpha\beta}^2) - \frac{T}{n}\log \mathrm{Tr}\exp(-\mathcal{H}_{\mathrm{eff}}) \tag{3}$$

where $d = \langle n^{a\alpha}\rangle$ is the mean density, $q_s = \langle S^{1\alpha} S^{2\alpha} n^{1\alpha} n^{2\alpha}\rangle$ is the spin overlap between two directly coupled replicas, $q_{\alpha\beta} = \langle S^{a\alpha} S^{a\beta} n^{a\alpha} n^{a\beta}\rangle$ and $p_{\alpha\beta} = \langle S^{1\alpha} S^{2\beta} n^{1\alpha} n^{2\beta}\rangle$ are respectively the overlap matrices between replicas with the same and with different 'real label', and $\mathcal{H}_{\mathrm{eff}}$ is the effective single-site Hamiltonian

$$\begin{aligned}\mathcal{H}_{\mathrm{eff}} = &-\left(\frac{\beta^2 J^2}{2} d + \beta\mu\right)\sum_{a\alpha} n^{a\alpha} - \beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} \sum_a S^{a\alpha} S^{a\beta} n^{a\alpha} n^{a\beta} \\ &- 2\beta^2 J^2 \sum_{\alpha<\beta} p_{\alpha\beta} S^{1\alpha} S^{2\beta} n^{1\alpha} n^{2\beta} - \beta^2 J^2 q_s \sum_\alpha S^{1\alpha} S^{2\alpha} n^{1\alpha} n^{2\alpha} - \beta\epsilon \sum_\alpha n^{1\alpha} n^{2\alpha}.\end{aligned} \tag{4}$$

In the replica symmetric approximation $q_{\alpha\beta} = q$ and $p_{\alpha\beta} = p$. We make the further approximation $q = p$, and obtain for the free energy

$$\begin{aligned}F = &-2T\log 2 + \frac{\beta J^2}{2}(d^2 + q_s^2 - 2q^2) - T\int \mathcal{D}z\, \log\left\{1 + 2\mathrm{e}^{\Xi}\cosh(\beta J\sqrt{q}\, z)\right. \\ &\left. + \mathrm{e}^{2\Xi+\beta\epsilon}\left[\mathrm{e}^{\Omega}\cosh^2(\beta J\sqrt{q}\, z) - \sinh\Omega\right]\right\}\end{aligned} \tag{5}$$

where $\Xi = \frac{\beta^2 J^2}{2}(d - q) + \beta\mu$, $\Omega = \beta^2 J^2 (q_s - q)$, and $\mathcal{D}z = \frac{\mathrm{d}z}{\sqrt{2\pi}}\,\mathrm{e}^{-z^2/2}$.

The physical states of the system will be given by the saddle points of the free energy, which are given by the equations

$$d = \int \mathcal{D}z \; \frac{e^{\Xi}\cosh(\beta J\sqrt{q}\,z) + e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \sinh\Omega\right]}{1 + 2e^{\Xi}\cosh(\beta J\sqrt{q}\,z) + e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \sinh\Omega\right]} \tag{6a}$$

$$q_s = \int \mathcal{D}z \; \frac{e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \cosh\Omega\right]}{1 + 2e^{\Xi}\cosh(\beta J\sqrt{q}\,z) + e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \sinh\Omega\right]} \tag{6b}$$

$$q = \int \mathcal{D}z \left(\frac{e^{\Xi}\sinh(\beta J\sqrt{q}\,z)\left[1 + e^{\Xi+\beta\epsilon+\Omega}\cosh(\beta J\sqrt{q}\,z)\right]}{1 + 2e^{\Xi}\cosh(\beta J\sqrt{q}\,z) + e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \sinh\Omega\right]} \right)^2 . \tag{6c}$$

Notice that the saddle points are neither maxima nor minima of the free energy, because F has to be minimized with respect to d and q_s, and maximized with respect to q. If $\epsilon = 0$ then $q_s = q$, $\Omega = 0$, and one obtains the saddle point equations of the uncoupled system. Differentiating the free energy F with respect to ϵ, we can evaluate the density overlap $q_d = \langle n^{1\alpha} n^{2\alpha} \rangle$,

$$q_d = -\frac{\partial F}{\partial \epsilon} = \int \mathcal{D}z \; \frac{e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \sinh\Omega\right]}{1 + 2e^{\Xi}\cosh(\beta J\sqrt{q}\,z) + e^{2\Xi+\beta\epsilon}\left[e^{\Omega}\cosh^2(\beta J\sqrt{q}\,z) - \sinh\Omega\right]}. \tag{7}$$

In the above expression we can put $\epsilon = \Omega = 0$, and find the expression of the density overlap for a system without coupling, which cannot be obtained directly from the free energy of the uncoupled system.

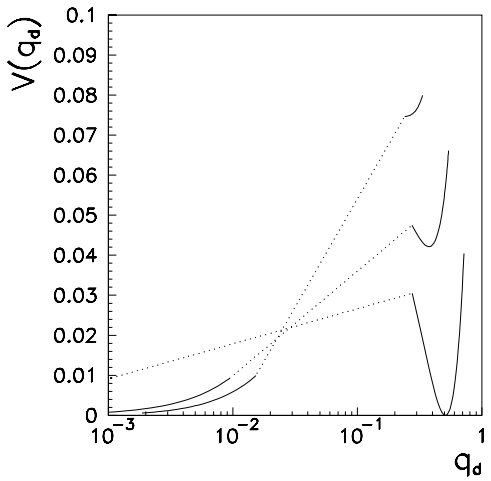

Figure 2. Effective potential as a function of the density overlap q_d, for chemical potential $\mu/J = -0.85$ and temperatures $T/J = 0.183$, 0.119 and 0.0538 (points marked with an asterisk in figure 1). The potentials for different temperatures are shifted so that the paramagnetic minimum is at $V = 0$. The dotted lines join the potentials at the same temperature, and are only a guide to the eye.

Now we want to compute the effective potential as a function of the density overlap q_d. The procedure to do so was previously sketched, and consists in evaluating $V(q_d) = \max_{\epsilon}[F(\epsilon) + \epsilon q_d]$. We evaluate $V(q_d)$ in three points of the phase space (marked by asterisks in figure 1). One point at the edge of the region in which spin-glass solutions of the saddle point equations exist, one on the line of first-order transitions, and one in between. The result is shown in figure 2. As soon as one enters in the region where spin-glass solutions

exist, a secondary minimum in the effective potential appears, signalling the existence of metastable states. We expect therefore that the dotted line of figure 1 will represent a line of purely dynamical transitions, below which ergodicity is broken and the relaxation function $\langle n_i(0)n_i(t)\rangle$ will not decay to its equilibrium value, which in the paramagnetic phase is the density squared, but will stick at the value given by the secondary minimum of the potential.

The presence of metastable states, and of a dynamical transition at a temperature higher than the static transition, in a model in which the low-temperature spin-glass phase is characterized by a full RSB, seems rather peculiar. It is reasonable to think that the usual picture, valid for p-spin models, according to which at the dynamical transition the phase space is split into an extensive number of valleys having all the same 'distance', i.e. the same mutual overlap, is modified in this case. Here, in fact, the spin-glass phase is characterized by a complex ultrametric structure, typical of the SK model. In particular, one may ask if in this case the gap ΔV in the effective potential can still be interpreted as a configurational entropy, i.e. the logarithm of the number of valleys in the configuration space. Finally, it would be interesting to understand how and to what extent this model can tell us something about real systems, that is structural glasses.

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