Random, thermodynamic and inverse first-order transitions in the Blume–Capel spin glass

Ulisse Ferrari and Luca Leuzzi

Dipartimento di Fisica, Università ‘La Sapienza’, and IPCF-CNR, UOS Roma, Piazzale Aldo Moro 2, I-00185 Rome, Italy
E-mail: ulisse.ferrari@roma1.infn.it and luca.leuzzi@cnr.it

Received 27 June 2011
Accepted 10 November 2011
Published 12 December 2011

Online at stacks.iop.org/JSTAT/2011/P12005
doi:10.1088/1742-5468/2011/12/P12005

Abstract. A class of model systems undergoing a glass transition with inversion of the fluid and glassy phase in temperature is investigated in order to qualitatively characterize the so-called inverse freezing phenomenon occurring in some complex glassy polymeric systems such as methylcellulose. The leading model we analyze is the spherical mean-field approximation of a spin-1 model with $p$-body quenched disordered interaction. Depending on temperature and chemical potential the system is found in a paramagnetic or in a glassy phase and the transition between these phases can be of a different nature. In the given conditions inverse freezing occurs. As $p = 2$ the glassy phase is replica-symmetric and the transition is always continuous in the phase diagram. For $p > 2$ the exact solution for the glassy phase is obtained by the one-step replica symmetry breaking ansatz. Different scenarios arise for both the dynamic and the thermodynamic transitions. These include (i) the usual random first-order transition (Kauzmann-like) preceded by a dynamic transition, typical of mean-field glasses, (ii) a thermodynamic first-order transition with phase coexistence and latent heat and (iii) a regime of inversion of static and dynamic transition lines. In the latter case a thermodynamic stable glassy phase, with zero configurational entropy, is dynamically accessible from the paramagnetic phase. Crossover between different transition regimes is analyzed by means of replica symmetry breaking theory and a detailed study of the complexity and of the stability of the static solution is performed throughout the space of external thermodynamic parameters.

Keywords: solvable lattice models, phase diagrams (theory), cavity and replica method, spin glasses (theory)
1. Introduction

In macromolecular compounds in solution, complex molecules or polymeric chains can fold into practically inactive conformations, displaying a negligible interaction with the surrounding system. The presence of inactive components can induce the existence of a fluid phase at a temperature below the temperature range at which the system is in a solid phase. This corresponds to the occurrence of an inverse transition, also called ‘melting upon cooling’, that is a reversible transition between a completely disordered isotropic fluid phase and a solid phase whose entropic content is greater than the entropy of the fluid. The solid phase can be crystalline or semi-crystalline, as in the compounds studied in [1, 2], or else amorphous, as in methylcellulose [3].

This effect can be reproduced and studied in statistical mechanical models on a lattice with bosonic spin-1 variables, where the holes \( s = 0 \) play the role of inactive states. In these models the fluid phase is the paramagnet and the solid phase is either a ferromagnet (no or weak disorder) or a spin glass (strong disorder). A prototype model with two-body interactions between bosonic spins is the Blume–Emery–Griffiths (BEG) model with ferromagnetic interaction [4]–[7] and its random magnetic implementation [8]–[21].
In the presence of quenched disorder the random BEG model is known to display both a continuous paramagnet/spin-glass phase transition and a first-order one (first order in the thermodynamic sense, i.e. with latent heat and a region of phase coexistence). Furthermore, inverse freezing takes place, with a spin glass at high $T$ and a paramagnet at low $T$. These properties have been observed in the mean-field approximation [20], where the self-consistent solution for the spin-glass phase is computed in the full replica symmetry breaking (RSB) Parisi ansatz [22]–[24] and on the cubic 3D lattice with nearest-neighbor couplings in systems exchanging two-body interactions as well [25,26]. The frustrated BEG model has been studied as well by means of numerical renormalization group techniques with apparently different results: on the Migdal–Kadanoff hierarchical lattice in 3D, it displays no inversion in the transition, nor a low $T$ discontinuity [27], whereas on the Wheatstone-bridge hierarchical lattice in dimension $\log 12/\log 2 \simeq 3.585$ the inversion seems to be present [28].

Mean-field spin-glass models with more than two-spin interactions, called $p$-spin models, are known to yield the so-called random first-order transition, i.e. a phase transition across which no internal energy discontinuity occurs but the order parameter (the Edwards–Anderson overlap $q_{EA}$) jumps from zero to a finite value. Their glassy phase is described by an ansatz with one RSB. In a cooling procedure, the thermodynamic transition is preceded by a dynamic transition due to the onset of a very large number of metastable states separated by high barriers. The phenomenology of the $p$-spin spin-glass systems is, in many respects, very similar to the one of structural glasses [29,36]. These models are, therefore, sometimes called mean-field glasses.

‘Very large’ means that the number of states $N$ grows exponentially with the size $N$ of the system: $N \sim \exp \Sigma N$, where the coefficient $\Sigma$ is the configurational entropy, also called complexity in the framework of quenched disordered systems. This is a fundamental property both in mean-field systems [29]–[33] and outside the range of validity of mean-field theory, e.g. in computer glass models [34,35], or, indirectly, by measuring the excess entropy of glasses in experiments, see, e.g., [36] and references therein.

‘High barriers’ means that the free energy difference between a local minimum in the free energy functional of the configurational space (also called free energy landscape) and a nearby maximum (or saddle) grows with $N$. That is, it diverges in the thermodynamic limit. This is a specific artifact of mean-field glasses. The thus induced dynamic transition corresponds to the transition predicted by another mean-field theory for the dynamics of supercooled liquids: the mode coupling theory [37]. The thermodynamic transition occurring at a lower temperature is, instead, the mean-field equivalent of the so-called Kauzmann transition in glasses, also known as the ideal glass transition, predicted by Gibbs and Di Marzio [38].

In order to understand melting upon cooling of a structural glass, we would like to investigate what happens to mean-field glasses when model features belonging to systems undergoing inverse freezing are introduced. This investigation was brought about initially by Sellitto in an another mean-field glass, with two-body interaction, i.e. the random orthogonal model (ROM) [39] with spin-1 variables [40]. In the present work we rather consider a multi-body interaction model: a $p$-spin interaction model, which can be built either using discrete Ising variables [41,42], soft spins [29] or spherical spins [31], the latter two being an approximation of Ising discrete variables that allows for an easier analytical treatment. We confirm the findings of [40] and deepen the analysis of the
amorphous phase, of the different kinds of transitions, as well as the complexity behavior in the transition region. We will see how non-trivial features will arise, among which is the crossover from a random to a standard thermodynamic first-order phase transition and the inversion of dynamic and static transitions, with the consequent possibility of accessing low energy glassy states without running into dynamic arrest into excited metastable states at high energy.

As a by-product, we also investigated the occurrence of complex eigenvalues in the stability analysis of the RSB solution and their connection to the actual thermodynamic stability of the phases displayed by the system.

2. Model

The model Hamiltonian that we will consider derives from

\[ \mathcal{H} = - \sum_{i_1 < \cdots < i_p} J_{i_1 \cdots i_p} s_{i_1} \cdots s_{i_p} + D \sum_i s_i^2 \]  

(1)

with \( s_i = 1, 0, -1 \). The couplings \( J \) are Gaussian independent identically distributed variables with probability distribution

\[ P(J_{i_1 \cdots i_p}) = \sqrt{\frac{N_{p-1}}{\pi J^2 p!}} \exp \left\{ - \frac{N_{p-1} J_{i_1 \cdots i_p}}{J^2 p!} \right\} . \]  

(2)

The coefficient \( D \), known as the crystal field in Blume–Capel (BC) models [4, 5], plays the role of a chemical potential for the empty sites (holes).

The \( p = 2 \) case was introduced in [8] and it has been studied subsequently throughout the years [9]–[20]. A preliminary study of the \( p \)-body case, in the \( p \to \infty \) limit, was presented in [43].

The spin-1 case can be translated into an Ising spin problem on a lattice gas. Indeed, if we rewrite \( s_i = \sigma_i n_i \) and crystal field \( D = D' + T \log 2 \), with \( \sigma = \pm 1 \) and \( n = 0, 1 \) we have

\[ \mathcal{H} = - \sum_{i_1 < \cdots < i_p} J_{i_1 \cdots i_p} \sigma_{i_1} \cdots \sigma_{i_p} n_{i_1} \cdots n_{i_p} + (D' - T \log 2) \sum_i n_i . \]  

(3)

We stress that the shift in chemical potential is necessary to keep the relative degeneracy of zero and non-zero values of the spins in the partition sum [44]. A different shift in \( D \) (or none) would actually define another model. Generally speaking a chemical potential transformation of the kind \( D = D' - T \log 2r \) will provide the Ising spin on a lattice gas model corresponding to a model with spin \(-1\) variables taking values \( s = 1 \) (or \( s = -1 \)) \( r \) times more frequently than the value 0. For example, \( r = 1/2 \) corresponds to \( s = 1, 0, 0, -1 \); \( r = 1 \) to the original case \( s = 1, 0, -1 \), cf equation (3); \( r = 4 \) to \( s = 1, 1, 0, -1, -1 \) and so on [6]. In the following we will address the variants with generic \( r \), as well.

In the Ising \( p \)-spin model, as \( p > 2 \), besides a random first-order transition (RFOT) between a paramagnet and a spin-glass phase in the 1RSB ansatz, a lower temperature phase transition is also expected to occur between the latter and a full RSB spin-glass phase. Indeed, this is what is known to occur in the \( D \to -\infty \) limit [42]. Since we are exclusively interested in the transition between a fluid and a (mean-field) glass, thus
1RSB-stable, we can simplify the computation by approximating the discrete spins with continuous real variables satisfying a global spherical constraint. As we will see later, this discrete to continuous simplification does not significantly affect the presence of an inverse transition, cf section 4.

As suggested in [45], we introduce, to this aim, the variable \( \tau = \sigma(2n-1) = \pm 1 \), such that \( n = (\sigma \tau + 1)/2 \), and eventually obtain the model Hamiltonian:

\[
\mathcal{H} = -\frac{1}{2p} \sum_{i_1 \cdots i_p} J_{i_1 \cdots i_p} (\sigma_{i_1} + \tau_{i_1}) \cdots (\sigma_{i_p} + \tau_{i_p}) + (D - T \log 2) \sum_{i=1}^{N} \frac{\sigma_i \tau_i + 1}{2}
\]

with

\[
\sum_{i=1}^{N} \sigma_i^2 = \sum_{i=1}^{N} \tau_i^2 = N.
\]

Applying RSB theory [22]–[24] we are going to investigate thermodynamics and complexity of the disordered model represented in equation (4).

3. Replicated free energy and order parameters

The replicated free energy, averaged over the distribution of disordered couplings, is

\[
f_n = -\frac{1}{nN\beta} \log \int \mathcal{D}Q \mathcal{D}T \mathcal{D}R \exp \left\{ -nN\beta G(\beta, D; Q, T, R) \right\}
\]

\[
- n\beta G = - (\beta D - \log 2) \sum_a R_{aa} + 1 - \frac{\beta^2}{4(p+1)} \sum_{a b} (Q_{ab} + T_{ab} + 2R_{ab})^p
\]

\[
+ \frac{1}{2} \ln \det \left( \frac{1}{2} (QT + TQ) - R^2 \right) + \frac{n}{2} \log \pi + n,
\]

\[
\mathcal{D}Q = \prod_{a<b}^{1,n} dQ_{ab} \quad \mathcal{D}T = \prod_{a<b}^{1,n} dT_{ab} \quad \mathcal{D}R = \prod_{a \leq b}^{1,n} dR_{ab}
\]

where we have inserted the three overlap matrices:

\[
NQ_{ab} = \sum_i \sigma_i^a \sigma_i^b, \quad NT_{ab} = \sum_i \tau_i^a \tau_i^b, \quad NR_{ab} = \sum_i \sigma_i^a \tau_i^b
\]

and, consequently, integrated over the spin variables. The saddle point, self-consistency, equations are

\[
Q_{ab} = T_{ab} = R_{ab}, \quad a \neq b
\]

\[
-\frac{1}{2} \left[ (QT - R^2)^{-1} \right]_{ab} = \frac{\beta D - \log 2}{4} \delta_{ab} - \frac{p\beta^2}{2(p+1)} (Q_{ab} + R_{ab})^{p-1}.
\]

From the free energy, cf equation (6), in the zero replica limit

\[
f = \lim_{n \to 0} G(\beta, D, Q^{\text{op}}, T^{\text{op}}, R^{\text{op}})
\]

doi:10.1088/1742-5468/2011/12/P12005

J. Stat. Mech. (2011) P12005
one derives all thermodynamic quantities, such as the density of filled-in sites:

\[ d = \frac{df}{dD} = \lim_{n \to 0} \frac{1}{n} \sum_a \frac{R_{aa} + 1}{2}; \]

(11)

the internal energy:

\[ u = \frac{\beta f}{\beta} = -Dd - \lim_{n \to 0} \frac{2\beta}{4(p+1)} \frac{1}{n} \sum_{ab} (Q_{ab} + T_{ab} + 2R_{ab})^p \]

(12)

and the entropy:

\[ s = d \log 2 + \frac{1}{2} \log \pi + 1 + \lim_{n \to 0} \frac{1}{2n} \left[ \frac{2\beta^2}{4(p+1)} \sum_{ab} (Q_{ab} + T_{ab} + 2R_{ab})^p + \ln \det (QT - R^2) \right]. \]

(13)

In order to compute the above expressions the precise shape of matrices \( Q, T \) and \( R \) has to be identified. There is no \( a \ priori \) method to deduce the correct form and one has to resort to an \textit{ansatz}.

The simplest one is the replica symmetric (RS) ansatz, where the discrete symmetry group \( S_n \), of permutation between replicas, holds for all two index quantities. This means that the elements of each overlap matrix \( M \) only take one value \( M_0 \) outside the diagonal and \( M \) can be parameterized as

\[ M_{ab} = (M_d - M_0)\delta_{ab} + M_0, \]

(14)

where \( \delta \) is the Kronecker delta. Replica symmetry always holds for one index parameter, because physical properties of a single replica must be identical for each replica. Indeed, all single index quantities, like the diagonal part of the \( R \) overlap matrix, are index-independent.

RS is not always self-consistent, though. Studying the fluctuations in the space of replica matrices around an RS solution for equations (8) and (9) one finds that, for \( p > 2 \), the glassy solution is not stable and one has to break the symmetry between replicas in order to find a self-consistent solution. To perform such stability analysis one needs the Hessian matrix. For our model it is computed in detail in appendix A. We will later report about the stability analysis of both the \( p = 2 \) case and the \( p > 2 \). Breaking the replica symmetry allows for different values in the off-diagonal elements of the overlap matrices. The symmetry can be broken step by step, allowing a further overlap value at each step and organizing replicas in clusters with a hierarchical structure [22, 23]. For our purpose one step turns out to be sufficient, leading to a \textit{one-step replica symmetry breaking} (1RSB) solution, in which a generic matrix takes the form

\[ M_{ab} = (M_d - M_1)\delta_{ab} + (M_1 - M_0)\epsilon_{ab} + M_0, \]

(15)

where \( \epsilon_{ab} = 1 \) if \( a \) and \( b \) belong to the same cluster of size \( m \) and \( \epsilon_{ab} = 0 \) otherwise.

doi:10.1088/1742-5468/2011/12/P12005
4. Thermodynamics for \( p = 2 \). Inverse freezing

For \( p = 2 \) the free energy evaluated in the RS ansatz is

\[
-2\beta \lim_{n \to 0} G_{RS} = -2(\beta D - \log 2)d + \frac{\beta^2}{2}(d^2 - q^2) + \frac{q}{\eta} + \log(\theta\eta) + \log(4\pi) + 2
\]  

(16)

where \( \theta = 1 - d \) and \( \eta = d - q \) are eigenvalues of the matrix \( QT - R^2 = Q^2 - R^2 \).

Self-consistency equations are

\[
\beta^2 q = \frac{q}{\eta^2} \tag{17}
\]

\[
\beta^2 \eta = \frac{\eta - \theta}{\theta \eta} + 2(\beta D - \log 2). \tag{18}
\]

In this two-body model case, the RS solution turns out to be marginally stable with respect to fluctuations in the space of replica parameters, as shown in appendix B. In particular, the lowest relevant eigenvalues of the Hessian, the so-called replicon, cf equation (B.13), is \( \Lambda_1^{(1)} = 0 \).

The self-consistency equation (17) admits \( q = 0 \) as a solution. This leads to a paramagnetic phase, characterized by a density \( d_{PM} \) (determined by imposing equation (18)) and whose free energy is

\[
-\beta f_{PM}^{RS}(\beta, D) = -(\beta D - \log 2)d_{PM} + \frac{\beta^2}{4}d_{PM}^2 + \frac{1}{2} \log[(1 - d_{PM})d_{PM}] + \frac{1}{2} \log(4\pi) + 1.
\]  

(19)

For low \( T \) and \( D \) the paramagnetic phase turns out to be unstable. In particular, equation (B.27) becomes negative and a new solution to equations (17) and (18) occurs with \( q > 0 \):

\[
d(T, D) = 1 - \frac{T}{2(1 - D + T \log 2)} \tag{20}
\]

\[
q(T, D) = 1 - T \left( \frac{3/2 - D + T \log 2}{1 - D + T \log 2} \right). \tag{21}
\]

This SG solution is stable in the RS ansatz in the whole region of the phase diagram where it exists, delimited by the transition line

\[
D_c(T) = 1 + T \log 2 - \frac{T}{2(1 - T)}. \tag{22}
\]

In figure 1 we plot the phase diagram for the model. At the transition the overlap parameter \( q \) grows continuously from 0, the paramagnetic and the spin-glass solutions coincide and the density crosses the transition continuously, as shown in figure 2. This defines a second-order transition, without latent heat or discontinuities in first-order derivatives. As shown in the figure, a re-entrance of the transition line points out the presence of inverse freezing.

\[1 \] Actually, there is a region in the \( D - T \) diagram with three solutions for \( d_{PM} \), but only one turns out to be stable. See also equation (40) with \( p = 2 \).
Figure 1. $T, D$ phase diagram of the $p = 2$ model case. Inset: the same diagram is shown for models with different values of the parameter $r = 1, 2, 4$ and 8, the ratio of the number of non-zero to zero values for the spin in the discrete counterpart of our spherical model. As $r$ increases the inverse transition region is enhanced.

Figure 2. Density behavior at $T = 0.4$ across the SG/PM transition for the $p = 2$ model. The paramagnetic density is shown (as a thin curve) also in its unstable phase.

Comparing with the more complicated discrete spin case, where the amorphous phase is stable only in the full RSB ansatz [20], we point out that the re-entrant behavior of the transition line is still there. Changing to continuous variables does not alter this property. The two systems differ in the nature of the amorphous phase and in the kind of transition (first order in the discrete spin case in the re-entrant region), but they both display inverse freezing.

As we mentioned above, in section 2, one can also easily switch models using Schupper–Shnerb variables [6, 7] controlling the degeneracy ratio $r$ between filled and empty sites in the original model with discrete variables. The effect of increasing $r$ is to increase the breadth of the interval in chemical potential for which inverse freezing takes place. In the inset of figure 1 we show the phase diagrams for some choices of $r$. 

doi:10.1088/1742-5468/2011/12/P12005
Random, thermodynamic and inverse first-order transitions

Finally, we stress that, besides $\Lambda_1^{(1)}$, cf equation (B.13), there are six more distinct eigenvalues of the stability Hessian, four of which are strictly real and positive. The other two, due to the $n \to 0$ limit, can be complex conjugated and develop an imaginary part. Their real part is always positive. We refer to appendix B for a detailed discussion. Here we only stress that, since the RS solution is exact for $p = 2$, the onset of imaginary eigenvalues is not a signature of a lack of consistency of the replica ansatz but an artifact due to the limit $n \to 0$ in the replica calculation. In figure 3 we plot the regions of the phase diagram in which imaginary stability eigenvalues occur.

4.1. Random matrix approach

To conclude the analysis of the $p = 2$ model we mention that, as shown in [45]–[47], the thermodynamics can be computed also with the method applied by Kosterlitz, Thouless and Jones [48] to the spherical Sherrington–Kirkpatrick model, that is the $D \to -\infty$ limit of the present model. The method consists in describing the model in terms of the variables $\hat{\sigma}_i^\lambda$ diagonalizing the interaction matrix:

$$\sum_j J_{ij} \hat{\sigma}_j^\lambda = J_\lambda \hat{\sigma}_i^\lambda.$$  

(23)

The partition function turns out to be

$$Z = \int dz \ pi^{N/2} e^{N \left\{ \frac{\beta}{2} (2z + D - T \log 2) - \log \beta/2 - 1/2 N \sum_\lambda \log[\Lambda_1(z)\Lambda_2(z)] \right\}}.$$  

(24)

where

$$\Lambda_1(z) = \frac{\beta}{2} \left( z - \frac{J_\lambda}{2} - \frac{D - T \log 2}{2} \right)$$  

(25)

$$\Lambda_2(z) = \frac{\beta}{2} \left( z + \frac{D - T \log 2}{2} \right).$$  

(26)
In the thermodynamic limit, the sum over the eigenvalues can be evaluated as an integration having as a measure Wigner’s semicircle law:

\[
\frac{1}{N} \sum_{\lambda} f(\lambda) \longrightarrow \int_{-2}^{2} dJ \rho(J) f(J) = \int_{-2}^{2} dJ \frac{1}{2\pi} \sqrt{4 - J} f(J).
\]  

(27)

Our replica calculation agrees with the result of Caiazzo et al [45]–[47].

5. Thermodynamics and complexity for the \( p > 2 \) model

The situation is far richer, and interesting, when more than two-body interactions among spin variables are considered. As \( p > 2 \), indeed, not only is the RS solution inconsistent in the SG phase (cf stability analysis in appendix B) but the exact one-step RSB solution yields different kinds of transitions, some of which are atypical in the framework of mean-field glasses. For \( p > 2 \) the 1RSB free energy is

\[
-\beta G^{\text{1RSB}} = -\left(\beta D - \log 2\right)d + \frac{\beta^2}{4} (p^p + (m - 1)q_1^p)
\]

\[
+ \frac{1}{2} \left( 2 \log 2 + \log \theta + \frac{m - 1}{m} \log \eta_0 + \frac{1}{m} \log \eta_1 \right),
\]

(28)

where we have used the expression of the eigenvalues of the \((Q^2 - R^2)\) matrix:

\[
\theta = 1 - d
\]

\[
\eta_0 = d - q_1
\]

\[
\eta_1 = d + (m - 1)q_1 - mq_0.
\]

We set \( q_0 = 0 \), because of the absence of an external magnetic field. Self-consistency equations are

\[
\phi(q_1) = \frac{q_1}{\eta_0 \eta_1}
\]

(32)

\[
\phi(d) - \phi(q_1) = \frac{\eta_0 - \theta}{\theta \eta_0} + 2(\beta D - \log 2)
\]

(33)

\[
z(y) = \frac{2}{\rho}
\]

(34)

where

\[
\phi(q) = \frac{\rho \beta^2}{2} q^{p-1}
\]

(35)

\[
y \equiv \frac{\eta_0}{\eta_1}
\]

(36)

and

\[
z(y) \equiv -2y \frac{1 - y + \log y}{(1 - y)^2}
\]

(37)

doi:10.1088/1742-5468/2011/12/P12005
is the Crisanti–Sommers function [31]. The analysis of the stability of the 1RSB solution is reported in section 5.4.2 and in appendix C.

The complexity functional, defined as the Legendre transform of the free energy functional, evaluated on the saddle point solution yielded by equations (32) and (33), logarithmically counts the number of metastable states [30]. It is

\[
\Sigma_{LT}(m, D, \beta) = \beta m^2 \frac{\partial}{\partial m} G(m, D, \beta, q^{\text{sp}}_1(m, D, \beta), \epsilon^{\text{sp}}(m, D, \beta)) = -\frac{m^2 \beta^2 (q^{\text{sp}}_1)^p}{4} - \frac{m \beta q^{\text{sp}} - \beta}{2} \log \frac{\eta^{\text{sp}}_0}{\eta^{\text{sp}}_1}.
\]

To determine the dynamic transition line \(T_d(D)\) one has to impose a maximal complexity (versus \(m\)) condition:

\[
\frac{\partial \Sigma_{LT}}{\partial m} = 0 \quad \leftrightarrow \quad \eta_1 = (p - 1) \eta_0
\]

in place of equation (34).

From the analysis of the paramagnetic solution (\(q_0 = q_1 = 0\), solving the self-consistency equation:

\[
\frac{d}{2} dp(1 - d) = T^2(2d - 1) + 2(TD - T^2 \log 2)(1 - d)d
\]

one finds a region in the \(T, D\) phase diagram where three solutions for the PM density \(d\) occur. One of them is always unstable, whereas the other two coexist between the spinodal lines. The latter can be expressed, in a parametric form in \(d\), by

\[
D = \sqrt{\frac{p}{p - 1}} \frac{d^{1+p/2}(d + p - 3dp + 2d^2p + 2(1 - d)^2d(p - 1) \ln(2r))}{2(1 - d) \sqrt{4d^2 - 4d + 1}}
\]

\[
T = \sqrt{p(p - 1)} \frac{d^{p/2}(1 - d)}{\sqrt{4d^2 - 4d + 1}}.
\]

The first-order transition line is, eventually, obtained by comparing the free energies of the two solutions. The existence of two PM phases is also found in the Blume–Capel ROM by Sellitto [40]. Moreover, two different fluid phases have been measured by means of neutron scattering and differential scanning calorimetry in a solution of \(\alpha\)-cycloextrin (\(\alpha\)-CD) and 4-methylpyridine (4MP) in water, a macromolecular compound undergoing melting upon cooling to a low temperature liquid from a crystal phase for high concentration of \(\alpha\)-CD in solution [2]. For low concentration of \(\alpha\)-CD, indeed, a high to low temperature liquid transition occurs, qualitatively akin to the PM\(^+\)/PM\(^-\) transitions occurring here and in Sellitto’s model. We will come back to these phases in the following.

In figures 4 and 5 we show the phase diagram for \(p = 3\), both for \(r = 1\) and 4. For \(r = 1\) no re-entrance of the thermodynamic transition line appears, as shown in figure 4\(^2\) but, increasing \(r\), inverse freezing is clearly reproduced, cf figure 5. The first-order PM\(^-\)/PM\(^+\) line is the thick dotted line and spinodal lines are plotted as thin dotted lines. Qualitatively distinct transition regimes are identified. We will dedicate a subsection to each one of them, starting from the most conventional one. As a reference we follow the phase diagram in figure 4 moving from small (and negative) to large (positive) values of the chemical potential of the holes.

\(^2\) This is in agreement with the lack of re-entrance in the discrete spin model in the \(p \to \infty\) limit [43].
Random, thermodynamic and inverse first-order transitions

Figure 4. $T$, $D$ phase diagram of the spherical $p = 3$-spin BC model with filled-in to empty sites ratio $r = 1$.

Figure 5. $T$, $D$ phase diagram of the spherical $p = 3$-spin BC model with filled-in to empty sites ratio $r = 4$. A re-entrance occurs in the first-order thermodynamic transition line.

5.1. Random first-order transition (RFOT)

For $D$ small enough our model displays the same behavior as the spherical $p$-spin model [31] and is an example of the well-known RFOT. At high temperature the system is in an ergodic paramagnetic phase. As it is cooled down, crossing a temperature $T_d$ it undergoes a dynamical arrest, despite the static order parameter $q_1$ is still null. Only at a lower temperature $T_s < T_d$ a thermodynamic phase transition occurs. Critical static
and dynamic lines are determined solving the equation systems (32)–(34) or (32), (33) and (39), respectively. For \( p = 3, r = 1 \), e.g. in the \( D, T \) phase diagram, they are

\[
D_s(T) = \frac{1.8794T^{1/3} - 2.49052T - 0.989769T^{5/3}}{1 - 1.42793T^{2/3}}
\]

(43)

\[
D_d(T) = \frac{21.6337T^{1/3} - 27.6822T - 11.5344T^{5/3}}{12.0 - 16.6407T^{2/3}}
\]

(44)

These curves are the \( m = 1 \)-lines for statics and dynamics, respectively represented in figures 4 and 5 by the thick full (dark gray) and dashed (light gray) lines. As one can observe in figure 6, crossing the dynamical temperature from high \( T \) values, a collection of high complexity SG states arises at high free energy values. Each one of these states has a free energy strictly greater than the free energy of the equilibrium state, namely the paramagnetic one. Indeed, from a strictly thermodynamic point of view, the stable state is the paramagnetic one, leaving each SG state as metastable. Decreasing further the temperature the system gains new states with lower free energy and complexity until, at \( T = T_s \), zero-complexity SG states appear, which turn out to yield the stable SG phase.

5.2. Thermodynamic first-order phase transition

Fluid–fluid transition. At \( (D_A, T_A) \simeq (0.73, 0.44) \) a first-order transition line starts developing in the PM phase, separating two distinct PM phases as \( T \) is lowered. The two phases are characterized by their density, which has a jump crossing the transition line. We call PM ± the paramagnetic phase at higher/lower density.

As in [40], the two PM phases have a different nature. For high chemical potential the energy cost per spin of being in the filled-in state \( (s_i = \pm 1) \) becomes unsustainable and the equilibrium phase is characterized by a fluid phase in which most of the sites...
Figure 7. Detail of the $D, T$ phase diagram with $r = 1$ with all significant critical points. $A$ is the critical point of the $\text{PM}^+/\text{PM}^-$ transition; $B$ is the merging point of the first-order $\text{PM}^+/\text{PM}^-$ with the first-order $\text{SG}/\text{PM}^-$ line; $E_{\text{d},\text{s}}$ is the limit of stability of the $\text{SG}$ (dynamic/static) solution along the $m_{\text{d},\text{s}} = 1$ line; $I$ is the point of dynamic–static inversion of the $m = 1$ lines (where the 1RSB solution is unstable) and $I_{\text{stab}}$ is the point of dynamic–static inversion in which the $\text{SG}$ solution is stable; $F_{\text{d},\text{s}}$ are the points of dynamic–dynamic and static–static $m$-lines crossing, in the region of replica instability.

are empty: $\text{PM}^-$. The density of filled-in sites of the $\text{PM}^-$ phase decreases with the temperature, leading to a sparse fluid at low $T$. This is the paramagnetic phase into which the glassy system might, possibly, ‘melt’ in an inverse freezing transition (as shown in figures 4 and 5, this actually occurs only for large enough $r$). For small positive values of $D$ (e.g. between approx. 0.7 and 1, as $T > 0.35$), a coexistence takes place with another $\text{PM}^+$ phase that is born discontinuously as a spinodal and whose density increases as $T$ decreases. We anticipate that the glassy 1RSB phase stems out of this solution, cf also figure 9. In figure 8 we show, for $D = 0, 0.75$ and 0.85, the density behavior for the two phases.

**Vitrification.** At $(D_B, T_B) \approx (0.77, 0.40)$ the first-order $\text{PM}^+/\text{PM}^-$ transition line merges with a first-order $\text{SG}/\text{PM}^-$ transition line $D_c(T)$, cf figure 7, and the thermodynamic transition to the $\text{SG}$ is not ‘random’ anymore but, rather, a standard first order, ruled by the Clausius–Clapeyron equation, cf, e.g., [20].

The $\text{SG}$ solution always departs from the high-density $\text{PM}^+$ phase, i.e. $\text{SG}$ and $\text{PM}^+$ belong to the same saddle point of equation (28), see, e.g., figure 9. For chemical potential values $D < D_B$ the thermodynamic transition to the $\text{SG}$ is still the RFOT analyzed above. In figure 9 we plot the temperature behavior of the free energies of the $\text{PM}^-$, $\text{PM}^+$ and $\text{SG}$ phases in three qualitatively different cases: for $D < D_A$, $D_A < D < D_B$ and $D > D_B$.

Along the $D_c(T)$ transition line, latent heat is taken from the glass in order to be transformed into a paramagnet, as we show in figure 10.

Around that line the $\text{SG}$ and the $\text{PM}$ phases coexist and compete. Beyond the B point, the RFOT line $T_s(D)$ becomes the SG spinodal since on the right side of the $D_c(T)$ line the glassy phase is metastable with respect to the $\text{PM}$ one. That is, the whole hierarchy of global and local glassy minima lies above the global thermodynamically dominant $\text{PM}$ minimum in the free energy landscape: $\Phi_{\text{SG}} > \Phi_{\text{PM}}$. 

doi:10.1088/1742-5468/2011/12/P12005
Figure 8. Density versus $T$ of the two paramagnetic phases in their coexistence region. Left: $D = 0$, only one fluid phase exists. Middle: $D = 0.75$, both phases thermodynamically dominant at the thermodynamic first-order transition (TFOT). Right: $D = 0.85$, the TFOT occurs as $PM^+$ is actually metastable with respect to the spin glass.

Figure 9. Free energy in the SG and PM phases in qualitatively different scenarios. The full curve represents $\Phi_{SG}$ in the 1RSB ansatz, $\Phi_{PM^+}$ and $\Phi_{PM^-}$ versus $T$ are plotted as dashed curves. $D = 0.7, 0.75, 0.8, 0.9$. Top left: at $D = 0.7 < D_A$, RFOT between $PM^+$ and SG, at $T_s$. Top right: RFOT between $PM^+$ and SG, at $T_s$ and TFOT between $PM^-$ and $PM^+$, at $T_c$, for $D = 0.75$ (larger than $D_A$ and smaller than $D_B$). Bottom left: TFOT between $PM^-$ and SG, at $T_c$, and RFOT between $PM^+$ and metastable SG, at $T_s$. Bottom right: RFOT between $PM^+$ and metastable SG, at $T_s$. 

doi:10.1088/1742-5468/2011/12/P12005
Random, thermodynamic and inverse first-order transitions

Figure 10. Left: latent heat at the first-order transition at $D = 1$ for the case $r = 1$. Inset: discontinuity of overlap $q_1$ (dotted line) and density $d$ (dashed line) across the same transition point at $T_c = 0.142$. Right: latent heat at $D = 1.2$ for the case $r = 4$, in the presence of inverse freezing the SG phase transforms into the PM (at lower entropy $\Delta s = s_{SG} - s_{PM} > 0$) one as $T$ decreases, taking heat from the thermal bath. Inset: the overlap $q_1$ (dotted line) is different from zero above the critical temperature $T_c = 0.146$. The density $d$ (dashed line) decreases discontinuously in the low $T$ PM phase.

This might seem weird in some respects. Indeed, in RSB theory, e.g. in the spherical $p$-spin model, the 1RSB–SG solution stems out of the PM phase, which is RS. At a given $T_s$ a 1RSB solution appears with a discontinuous jump in $q_{EA}$ and no discontinuity in the free energy. As $T < T_s$, the SG free energy is larger than the PM free energy but it is the one which is thermodynamically stable because of the $n - 1, n - m$ or $m - 1$ factors present in the free energy expression equation (28) whose sign is inverted in the $n \to 0$ limit. This implies that looking for a minimal free energy at a finite integer number of replicas corresponds to looking for the maximal of the Parisi free energy. In our case, in fact, the SG–1RSB phase stems out of a PM (PM$^+$) phase, as shown in figure 9. However, it competes with another phase PM$^-$, corresponding to a different saddle point of equations (28), that does not transform into an SG and whose free energy does not involve overlap terms and, consequently, coefficients do not change sign in the replica calculation.

As a homogeneous selecting rule, we can thus apply the minimal free energy principle for all competing solutions with $n > 1$ and let $n \to 0$ only after the choice of the dominant stable phase has been done. To better exemplify this, we plot in figure 11 the RS-approximated SG solution at finite $n$ for different values of $n$ and we compare it with both the free energies of PM$^-$ and PM$^+$. For $n > 1$ the free energy of the SG–RS solution crosses the PM$^-$ free energy for $T$ lower than the transition temperature between the two PM phases, signaling the presence of a transition between the PM$^-$ and the SG. The dominant phase is the one of least free energy, i.e. the SG phase. As $n$ decreases the critical

doi:10.1088/1742-5468/2011/12/P12005
Figure 11. Analysis of free energy in temperature at finite $n = 0, 0.5, 1, 1.5$ and $2$ in the RS approximation. The full curve is the SG solution in the zero replica limit. The dashed curves are finite $n$ SG solutions. For $n = 1$ the SG free energy coincides with the PM$^+$ free energy. Each one of the SG curves crosses the free energy curve of the PM$^-$ phase signaling a first-order phase transition between the PM$^-$ phase, dominant at high $T$ and the SG phase (dominant at low $T$). Since the SG free energy is computed in the RS ansatz, the exact free energy is a little bit larger and the crossing point is at slightly smaller $T$.

temperature decreases until, for $n = 1$, the SG free energy turns out to be equal to the PM$^+$ one. As $n < 1$ the SG free energy shifts further towards small temperature but the thermodynamic order relationship with the free energy of the PM$^-$ phase is unchanged. Breaking the replica symmetry on the same SG phase leads to a higher free energy and shifts the first-order critical temperature towards smaller $T$. This does not affect the order relationship with respect to the other self-consistent solution, i.e. the PM$^-$ phase.

5.3. Dynamic–static inversion: disappearing of dynamic arrest

As the chemical potential increases, the temperature interval between $T_n(D)$ and $T_d(D)$ decreases down to zero at $T_n(D_I) = T_d(D_I) = T_I = 0.3739$, with $D_I = 0.8905$. For larger $D$, what we called so far the ‘dynamic’ line and the static line invert their positions in $T$. Beyond this point the term ‘dynamical transition’ becomes, actually, misleading. Usually, in the $p$-spin model [31], coming from high temperature, the appearance of metastable states coincides with the occurrence of a maximum of the complexity function, cf equation (38). This is for two reasons: (i) because only metastable states with an exponentially large degeneracy in free energy (i.e. an extensive complexity) can trap the dynamics and (ii) because those metastable states are the first where the system can relax to, cooling from high temperature (see figure 6).

For $D > D_I$, the behavior of the complexity function is, instead, different as we exemplify in figure 12. No exponentially large multitude of excited metastable states
appear when cooling towards the SG static transition and, therefore, no dynamic arrest into a metastable glassy state takes place for $T > T_s(D)$. Cooling further down below $T_s(D)$, the complexity function grows from zero, at $T_s$, to a maximum at a temperature coinciding with the continuation of the $T_d(D)$ line. $T_d$ is then the largest temperature at which the maximal complexity is first reached in a cooling procedure.

According to the above-mentioned behavior of the complexity, cf figure 12, one might conjecture that the lowest equilibrium glassy states are dynamically accessible at the static transition point by means of a quench from high $T$ exactly to $T_s$\(^3\). Along a further (slow) cooling the system could remain in the lowest glassy states while excited glassy states would develop at higher free energy. One can, furthermore, think about quenching to a $T_d < T < T_s$: this would initially lead the system to an excited state at the free energy value of maximum complexity at that $T$, lower than the absolute complexity maximum for the model. One might, thus, have the chance of investigating weak ergodicity breaking and lack of time translational invariance of two time quantities in a dynamics substantially influenced by the free energy landscape change with $T$. We can expect aging on two time observables both at $T_s$ (similarly to what happens in spin-glass models with continuous transitions) and for $T < T_s$, the latter case being quite unusual. Indeed, slowly cooling the system further, new threshold states will arise at higher free energy and predicting the dynamics of the system is far from trivial.

For quenches at and below $T_d$, finally, all quenches would lead to the highest possible thresholds states as in ordinary 1RSB systems below $T_s$ and both weak ergodicity and TTI breaking, as well as aging, is expected to occur as in ordinary systems with 1RSB (e.g.

\(^3\) This is not strictly true because the RFOT static transition line is actually a spinodal, since the thermodynamic dominant phase is PM beyond the $D_c(T)$ line. This implies that only quenches from a given subset of initial conditions would lead to the glassy phase, avoiding the paramagnet.

\[ \text{Figure 12. } \Sigma(f) \text{ for } T = 0.35 \text{ at different values of } D \text{ below the static transition.} \]
Figure 13. $T(D)$ lines of constant $m$ (from static equations). As $D$ is large enough they bend and cross each other. Left: complete behavior of $m$ lines. Right: only curves along which the compressibility is non-negative are plotted. An equivalent situation occurs for the dynamic $m$ lines. The thick continuous curve is the line where complex stability eigenvalues acquire negative real part: solutions on the right-hand side of the stability line are rejected.

spherical and Ising $p$-spin or ROM). To go beyond qualitative speculations, a detailed dynamic analysis is needed, that goes beyond the scope of the present work.

Eventually, to be more precise about the transition and spinodal lines, it can be seen from the complete stability analysis, cf appendix C, that for $D > D_{Ed} = 0.8737$, slightly smaller than $D_I$, the SG dynamic solution spanned along the $m = 1$-line turns out to display a couple of complex conjugated eigenvalues with negative real part. This implies that for $D \geq D_E$ the first thermodynamically stable SG solution occurs with the static parameter $m < 1$ and zero complexity for the excited states. The static–dynamic inversion then occurs, self-consistently, for values of $m < 1$, at $D_{I_{stab}} = 0.877$, $T_{I_{stab}} = 0.377$.

5.4. $m$-lines inversion, compressibility and replica stability

As one can see from figure 13, solving equations (32)–(34) [else (39)], and following solutions at fixed $m$ in the $D, T$ plane, each $T_m(D)$ curve (‘$m$ line’) develops a maximum and $T_m(D)$ lines at different $m$ values cross. This leads to an ambiguity: there is a region in the phase diagram in which in each point two different solutions of equations (32)–(34) occur. A criterion is then required to select the correct (metastable) phase in each point and, furthermore, a way to mark the spinodal of the SG. The solution comes from the positiveness of the compressibility $\kappa$ and from the complete analysis of the stability of the 1RSB solution in the replica space. Moreover, as we already mention, the $m$-line inversion complies with the fact that the spinodal SG lines (both dynamic and static) will cease to be lines of constant $m = 1$.

5.4.1. Compressibility. As a thermodynamic quantity the compressibility is usually defined as

$$k = - \frac{\partial \log V}{\partial p} \bigg|_T.$$  \hfill (45)
In our model, where the role of the pressure is played by the chemical potential $D$ and the inverse specific volume is the density of filled-in states $d$, the compressibility, cf figure 14, is

$$k = d \frac{\partial d^{-1}}{\partial D} \bigg|_T = -\frac{1}{d} \frac{\partial d}{\partial D} \bigg|_T = -\frac{1}{d} \frac{\partial d}{\partial m} \bigg|_T \frac{\partial m}{\partial D} \bigg|_T$$

(46)

where the last equality comes from Fubini’s implicit function theorem. Obviously, solutions with negative compressibility are unphysical and have to be discarded. At fixed $T$ the value $m = \tilde{m}$ yielding the zero point of the compressibility is given by

$$\left. \frac{\partial m}{\partial D} \right|_{m=\tilde{m}} = 0$$

(47)

using, for example, equation (33) for the $D(m)$ dependence. Beyond $\tilde{m}(T)$ the compressibility turns negative and that solution will be rejected. This kind of ‘selection rule’ has to be used for both the static and the dynamic $m$ lines.

The positiveness of $\kappa$ is certainly a necessary condition for thermodynamic stability. On top of that we anticipate that, from the replica stability analysis, we found a small region of the phase diagram where $\kappa > 0$ but the real part of a couple of complex conjugated eigenvalues among $\Lambda_{2,1}$, or among $\Lambda_{3,1}$ of the Hessian in the replica space for the 1RSB ansatz, cf equations (C.18) and (C.23), is negative (see also the right panel of figure 13). The spinodal lines plotted in figures 4 and 5 are drawn taking the latter observation into account. See also the right panel of figure 13.

The previous discussion implies that the dynamic SG spinodal is the $m = 1$ line on the left side of the point $F_d$, $(D_{F_d} = 0.98, T_{F_d} = 0.33)$ and a line of decreasing $m$ on the right side. Also the static SG spinodal undergo the same change at the point $F_s$ $(D_{F_s} = 1.03, T_{F_s} = 0.32)$. We remark, however, that this change in behavior arises for $D > D_I_{\text{stab}}$, where the $m = 1$ line cease to be stable in the replica space and $D > D_I$, after that the static–dynamic inversion occurs.

doi:10.1088/1742-5468/2011/12/P12005
5.4.2. Stability of 1RSB solution. In order to determine the above phase diagram it has been necessary to study the stability of the 1RSB solution in the $T, D$ plane. In appendix C we show the details of our analysis. The phenomenology looks similar to the RS case with both real and complex eigenvalues. The stability of the SG solution is ruled by $\Lambda^{(3)}_{1,1}$, the lowest real eigenvalue of the matrix $H_{11}$, cf equation (C.10). Evaluated on the static SG solution it is always positive, thus, according to our analysis, the static SG–1RSB solution is always stable. If, however, the static equation (34) is not imposed and the parameter $m$ is, thus, left undetermined, the positiveness of $\Lambda^{(3)}_{1,1}$ is equivalent to the condition

$$\eta_1 > (p - 1)\eta_0$$

(48)

and the equality $\Lambda^{(3)}_{1,1} = 0$ turns out to coincide with the dynamical condition equation (39). The other real eigenvalues are positive in the whole phase diagram.

In the region of phase coexistence, near the SG spinodal, the stability analysis actually reveals more subtle features. Indeed, as in the $p = 2$ case, cf section 4, complex eigenvalues are present and some of them develop a negative real part. In particular, solutions with negative compressibility always yield an imaginary eigenvalues with negative real part. Moreover, in a small region of the $T, D$ plane solutions with $\kappa \gtrsim 0$ also display complex eigenvalues, $A_{2,1}$ or $A_{3,1}$, cf equations (C.18) and (C.23) with negative real part. As anticipated, in determining the phase diagram we have thus rejected solutions with negative replica eigenvalues, including all those with negative compressibility.

6. Conclusions

At the level of mean-field theory, we have been analyzing a family of models mixing the properties of (i) Blume–Capel models with quenched disorder and (ii) spin-glass models with many-body ($p > 2$) interactions. The first ones are known to reproduce the inverse freezing to a glassy phase occurring, for example, in complex frustrated macromolecular compounds in solution [3] and display first-order thermodynamic phase transitions even in the presence of strong disorder. The latter yield most of the basic features of the standard folklore of glassy systems and are often refereed to as mean-field glasses. Our aim has been to investigate what happens to the dynamic arrest, displayed in mean-field glasses, as a system undergoes an inverse thermodynamic transition.

We have been studying the problem by means of replica theory for the two qualitatively distinct cases with $p = 2$ and $p > 2$, looking at the thermodynamics and at the dynamic properties that can be inferred from the static analysis of the complexity functional. The model approximation used is to pass from discrete spin-1 variables to spherical ones (i.e. continuous variables with an overall ‘spherical’ constraint) keeping the original probabilistic relationship between states of the discrete spin: $r \equiv [\# \text{ of times } s = 1]/[\# \text{ of times } s = 0]$. This allows for thoroughly analytical computation of complicated physical quantities. For what concerns the property of inverse freezing, this is left unchanged by the softening of the spins that we assumed as working hypothesis: for $p = 2$ the re-entrance is there for $r = 1$ as in the original random BEG model [20]; for $p > 2$ no re-entrance is found for $r = 1$, consistently with the spin-1 study of the $p \to \infty$ case by Mottishaw [43].

We have been mainly focusing on the case $r = 1$, i.e. the spherical formulation of the original BC model. We have considered, as well, model cases with different $r$ values.

doi:10.1088/1742-5468/2011/12/P12005
Indeed, in those cases where the system with $r = 1$ does not show inverse freezing, a simple variant of the model for larger $r$ is suitable to describe such a phenomenon.

The external parameters driving possible transitions are the temperature and a chemical potential for the empty states of the spin-1 variables, the so-called ‘crystal field’ $D$. For $D = -\infty$ one has no holes and the limit of the model is the spherical spin glass. In that limit, in the $p = 2$ case [48] the spin-glass phase is described by a replica symmetric ansatz and the transition turns out to be always continuous, whereas as $p > 2$ the RS solution is unstable and the right physics is described by a one-step replica symmetry breaking phase [31]. On top of it the transition is not continuous (at zero external magnetic field) in the order parameter and it is often refereed to as random first order.

Moving to larger positive values of the field $D$ the behavior for the $p > 2$ is, however, drastically modified and interesting less standard phenomena can be described.

- Two paramagnetic phases show up and a first-order PM$^+/PM^-$ phase transition line is found. Such fluid–fluid transition was previously found in the theoretical work of Sellitto [40] in the spin-1 ROM and has been experimentally detected in a solution of $\alpha$-CD and 4MP in water [2]. In the present work we could characterize the nature of both fluid phases and their transition. Indeed, their density behavior in temperature turns out to be opposite: as $T$ decreases, $d_{PM^+}(T)$ increases and $d_{PM^-}(T)$ decreases, allowing for an almost empty fluid at low $T$. This is the precursor ingredient that can possibly (not always, depending on $r$) leads to inverse freezing for large enough $D$. Moreover, PM$^-$ competes with the other phase, causing a thermodynamic first-order phase transition between PM$^-$ and PM$^+$ that continues into a transition between PM$^-$ and SG at lower $T$, as PM$^+$ transforms into the SG by means of a random first-order phase transition.

- Besides the standard RFOT, indeed, we find that, for large enough $D$, a first-order thermodynamic phase transition between the spin glass and the paramagnetic (PM$^-$) phase takes over, with latent heat and jumps in density and overlap order parameter. The spin glass becomes metastable with respect to the paramagnet and the RFOT line plays the role of the spin-glass spinodal. Experiments on methylcellulose [3] or similar compounds possibly undergoing inverse freezing might help clarifying the actual nature of the transition.

- Analyzing in detail the structure of the solutions in the phase diagram and their stability properties, we find that the spin-glass phase can be approached, in given regions (approximately for large $D$ and low $T$), without incurring in a dynamic arrest, unlike in the standard $p$-spin. Furthermore, the spin-glass solution along the transition line displays values of the replica symmetry breaking parameter $m$ less than one. The study of the complexity functional in those regions of the phase diagram induces us to conjecture that in a cooling experiment lowest glassy minima of the free energy landscape develop first, while excited metastable glassy states only arise as temperature is further decreased. Were the conjecture verified, the model could provide a test-bed to follow dynamics along given paths of the phase diagram into the deep glassy phase without being stuck in the threshold states. A dynamic analysis is beyond the scope of the present work and will be addressed elsewhere.
Eventually, we also mention that we have been solving a long-standing technical issue about the occurrence and the role played by complex stability eigenvalues of the RSB solution [9,11,14]. Performing a complete stability analysis of both RS and 1RSB solutions for any \( p \) model, we explicitly verified that the occurrence of an imaginary part of replica eigenvalues is not a signal of instability, but just an artifact of the replica \( n \to 0 \) limit.

Acknowledgments

The authors thank Andrea Crisanti and Giorgio Parisi for stimulating discussions. The research leading to these results has received funding from the Italian Ministry of Education, University and Research under the Basic Research Investigation Fund (FIRB/2008) program/CINECA grant code RBFR08M3P4.

Appendix A. Hessian of the spherical \( p \)-spin Blume–Capel model

In order to verify the stability of a saddle point calculation, the positiveness of the fluctuation matrix evaluated on the stationary solution has to be checked. This Hessian matrix is constructed as the second-order variation of the free energy potential (6) with respect to the three overlap matrices (7) and, indeed, depends on two couples of indices:

\[
H(G)^{O,O'}_{ab,cd} = \frac{\partial^2 G}{\partial O_{ab} \partial O'_{cd}}, \quad O, O' = Q, S, T. \tag{A.1}
\]

In detail the elements are

\[
\begin{align*}
\frac{\partial G^2}{\partial Q_{ab} \partial Q_{cd}} &= -B_{ab} \delta_{ac} \delta_{bd} + \frac{1}{8} [A_{a,c}(TAT)_{bd} + 2(TA)_{a,c}(AT)_{bd} + (TAT)_{a,c}A_{bd}] \\
\frac{\partial G^2}{\partial Q_{ab} \partial T_{cd}} &= -B_{ab} \delta_{ac} \delta_{bd} + \frac{1}{8} [A_{a,c}(TAQ)_{bd} + (QA)_{ac}(AT)_{bd} \\
&\quad + (AT)_{ac}(AQ)_{bd} + (TAQ)_{ac}A_{bd}] - \frac{1}{4} (A_{bd}\delta_{ac} + A_{ac}\delta_{bd})
\end{align*}
\]

\[
\begin{align*}
\frac{\partial G^2}{\partial Q_{ab} \partial R_{cd}} &= -2B_{ab} \delta_{ac} \delta_{bd} - \frac{1}{4} [A_{a,c}(TAR)_{bd} + (RA)_{ac}(AT)_{bd} \\
&\quad + (AT)_{ac}(AR)_{bd} + (TAR)_{ac}A_{bd}]
\end{align*}
\]

\[
\begin{align*}
\frac{\partial G^2}{\partial T_{ab} \partial Q_{cd}} &= -B_{ab} \delta_{ac} \delta_{bd} + \frac{1}{8} [A_{a,c}(TAQ)_{bd} + (QA)_{ac}(AT)_{bd} \\
&\quad + (AT)_{ac}(AQ)_{bd} + (TAQ)_{ac}A_{bd}] - \frac{1}{4} (A_{bd}\delta_{ac} + A_{ac}\delta_{bd})
\end{align*}
\]

\[
\begin{align*}
\frac{\partial G^2}{\partial T_{ab} \partial T_{cd}} &= -B_{ab} \delta_{ac} \delta_{bd} + \frac{1}{8} [A_{a,c}(QAR)_{bd} + 2(QA)_{ac}(AQ)_{bd} \\
&\quad + (AQ)_{ac}(AR)_{bd} + (QAR)_{ac}A_{bd}]
\end{align*}
\]

\[
\begin{align*}
\frac{\partial G^2}{\partial T_{ab} \partial R_{cd}} &= -2B_{ab} \delta_{ac} \delta_{bd} - \frac{1}{4} [A_{a,c}(TAR)_{bd} + (RA)_{ac}(AT)_{bd} \\
&\quad + (AQ)_{ac}(AR)_{bd} + (QAR)_{ac}A_{bd}]
\end{align*}
\]

\[
\begin{align*}
\frac{\partial G^2}{\partial R_{ab} \partial Q_{cd}} &= -2B_{ab} \delta_{ac} \delta_{bd} - \frac{1}{4} [A_{a,c}(TAR)_{bd} + (RA)_{ac}(AT)_{bd}]
\end{align*}
\]
Random, thermodynamic and inverse first-order transitions

\[ \frac{\partial G^2}{\partial R_{ab} \partial T_{cd}} = -2B_{ab} \delta_{ac} \delta_{bd} - \frac{1}{4} [A_{ac} (QAR)_{bd} + (RA)_{ac} (AQ)_{bd}] + (AR^2)_{ac} (AQ)_{bd} \]

\[ = -4B_{ab} \delta_{ac} \delta_{bd} + \frac{1}{2} [A_{ac} (RAR)_{bd} + 2(RA)_{ac} (AR)_{bd}] + (RAR)_{ac} A_{bd} \]

\[ \frac{\partial G^2}{\partial R_{ab} \partial R_{cd}} = -2B_{ab} \delta_{ac} \delta_{bd} - \frac{1}{2} \left[ A_{ac} (RAR)_{bd} + 2(AQ)_{ac} \delta_{ac} + A_{ac} \delta_{bd} \right] \]

where

\[ A_{ab} = (QT - R^2)_{ab} \]

\[ B_{ab} = \frac{\beta^2 p(p - 1)}{26} \left( \frac{Q_{ab} + T_{ab} + 2R_{ab}}{4} \right)^{p-2}. \]

To check its positiveness of the Hessian, one needs to compute and determine the sign of all the eigenvalues of its action on fluctuation matrices (\( \delta o \)'s):

\[ \Lambda \delta o_{ab} = \sum_{cd} \left( \frac{\partial^2 G}{\partial O_{ab} \partial Q_{cd}} \delta q_{cd} + \frac{\partial^2 G}{\partial O_{ab} \partial T_{cd}} \delta t_{cd} + \frac{\partial^2 G}{\partial O_{ab} \partial R_{cd}} \delta r_{cd} \right) \]

\[ = -B_{ab} \delta o_{ab} + \frac{1}{2} \sum_{cd} \left( \sum_{o'} \frac{\partial^2}{\partial O_{ab} \partial O_{cd}} \log |A| \right) \delta o_{cd}. \]  

\[ (A.4) \]

In order to solve equation (A.4), a set of \((3n^2 - n)/2\) coupled equations, one needs to find a way to project the system on proper subspaces, which allows us to translate the calculation to an usual eigenvalues problem.

**Appendix B. Stability of the RS solution**

In order to understand the appearance of complex eigenvalues, we start the stability analysis retaining \( n \) finite. In the RS ansatz the matrices (A.2) and (A.3) become

\[ A_{ab}^{-1} = \frac{1}{4\theta \eta} \delta_{ab} - \frac{q}{4\theta \eta \eta_1} \equiv x \delta_{ab} + w \]  

\[ x \equiv \frac{1}{4\theta \eta} \]  

\[ w \equiv -\frac{1}{4\theta \eta \eta_1} \]  

\[ B_{a \neq b} = \frac{1}{32} \phi'(q) = \frac{\beta^2 p(p - 1)}{26} q^{p-2} \equiv B_q, \]  

\[ B_{a = b} = \frac{1}{32} \phi'(d) = \frac{\beta^2 p(p - 1)}{26} d^{p-2} \equiv B_d \]  

\[ (B.1) \]

\[ (B.2) \]

\[ (B.3) \]

\[ (B.4) \]

\[ (B.5) \]

doi:10.1088/1742-5468/2011/12/P12005

24
where \( \theta = 1 - d \), \( \eta = d - q \) and \( \eta_1 = d - (1 - n)q \), with \( \eta_1 \rightarrow \eta \) if \( n \rightarrow 0 \). The parameter \( x \) is always positive. For later convenience, we define:

\[
D_{++} \equiv x^2(\eta + \theta)^2; \quad H_{++} \equiv xw[\eta^2 + 4\theta^2 + \eta(4\theta - \eta_1)]; \quad (B.6)
\]

\[
D_{+-} \equiv (\eta + \theta)(\eta - \theta); \quad H_{+-} \equiv xw(\eta^2 - 4\theta^2 - \eta\eta_1); \quad (B.7)
\]

\[
D_{--} \equiv (\eta - \theta)^2; \quad H_{--} \equiv xw(\eta^2 + 4\theta^2 - \eta(2\theta + \eta_1)). \quad (B.8)
\]

**Projection on subspace** \( S_1 \)

Fluctuations that involve the overlap of one replica with the others, are selected by projecting the Hessian (A.1) in the subspace \( S_1 \) defined by

\[
\delta r_{a,a} = 0, \quad \sum_{\gamma} \delta q_{a,\gamma} = 0
\]

with dimension \( d(S_1) = d_{\text{tot}} - 4n = 3n(n - 3)/2 \). This is called a replicon subspace and in \( S_1 \) the Hessian matrix reduces to:

\[
H_1 = \begin{pmatrix}
\frac{1}{2}D_{++} - B_q & \frac{1}{2}D_{++} - \frac{\eta}{2} - B_q & -D_{+-} - 2B_q \\
\frac{1}{2}D_{++} - \frac{\eta}{2} - B_q & \frac{1}{2}D_{++} - B_q & -D_{+-} - 2B_q \\
-D_{+-} - 2B_q & -D_{+-} - 2B_q & 2D_{--} + x - 4B_q
\end{pmatrix}
\]

\[(B.9)\]

displaying no explicit \( n \) dependence. The characteristic polynomial, evaluated on the SG solution, is

\[
P[H_1] = \left( \Lambda - \frac{x}{2} \right) (\Lambda^2 - b_1 \Lambda + c_1) \quad (B.10)
\]

\[
b_1 = \frac{3(\eta^2 - (p - 2)\theta^2)}{16\eta^2\theta^2} \quad (B.11)
\]

\[
c_1 = -\frac{p - 2}{8\eta^2\theta^2}. \quad (B.12)
\]

**Interaction with** \( p = 2 \). \( p = 2 \) \( c_1 = 0 \), \( b_1 > 0 \): two eigenvalues will be positive and one will be zero:

\[
\Lambda_1^{(1)} = 0 \quad (B.13)
\]

\[
\Lambda_1^{(2)} = \frac{3}{16\theta^2} > 0 \quad (B.14)
\]

\[
\Lambda_1^{(3)} = \frac{1}{8\theta\eta} > 0. \quad (B.15)
\]

We have marginal stability of the RS–SG solution.
Interaction with $p > 2$ and replica symmetry breaking. If $p > 2$, instead, $c_1 < 0$, leading to a negative zero of the polynomial and causes the instability of the RS–SG solution. As $p > 2$ one has to resort to a more complicated ansatz, the 1RSB scheme of computation, whose stability will be analyzed in the following appendix C. We now continue the analysis of the RS fluctuations in other subspaces.

Projection on subspace $S_2$

Fluctuations of the cluster of replicas are selected by projecting in $S_2$, defined as

$$
\sum_{\gamma} \delta r_{\gamma, \gamma} = 0, \quad \sum_{\gamma, \delta} \delta q_{\gamma, \delta} = 0
$$

with $d(S_2) = 4n - 4$. In $S_2$ the Hessian reduces to

$$
H_2 = H'_1 + \begin{pmatrix}
\frac{n-2}{8} H_{++} & \frac{n-2}{8} (H_{++} - 2w) & -\frac{n-2}{8} H_{+-} & -\frac{n-2}{8} H_{+-} \\
\frac{n-2}{8} (H_{++} - 2w) & \frac{n-2}{8} H_{++} & -\frac{n-2}{8} H_{+-} & -\frac{n-2}{8} H_{+-} \\
-\frac{1}{4} H_{+-} & -\frac{1}{4} H_{+-} & \frac{1}{2} H_{--} + w & \frac{1}{2} H_{--} + w \\
-\frac{1}{4} H_{+-} & -\frac{1}{4} H_{+-} & \frac{1}{2} H_{--} + w & \frac{1}{2} H_{--} + w
\end{pmatrix}
$$

where

$$
H'_1 := \begin{pmatrix} H_1 & 0 \\ 0 & \Lambda_4 \end{pmatrix}
$$

with

$$
\Lambda_2^{(4)} = -4B_3 + x + 2D_{--}.
$$

For generic $n$, apart from $n = 4$, $H_2$ is not symmetric, so the matrix can have complex eigenvalues. The characteristic polynomial of the $H_2$ matrix, evaluated on the SG solution, is

$$
P[H_2](\Lambda) = \left( -\Lambda + \frac{x}{2} + \frac{n-2}{4} w \right) \left[ -\Lambda^3 + a_2(n)\Lambda^2 - b_2(n)\Lambda + c_2(n) \right].
$$

In the limit $n \rightarrow 0$, the coefficients are

$$
a_2 = -2w\eta^2 x^3
$$

$$
b_2 = -wx + 6x^4\eta^4
$$

$$
c_2 = 5x^2\eta^2 - 2wx\theta^2.
$$

Interaction with $p = 2$. For the case $p = 2$, a numerical study ensures that all the solutions of the characteristic polynomial are real positive or complex conjugated with a positive real part. The region of the $(D, T)$ plane where the polynomial has complex zeros (shown in figure 3) can be determined by imposing

$$
\frac{u^2}{4} + \frac{v^3}{27} > 0
$$

where (in terms of the polynomial coefficients)

$$
u = \frac{2a_3}{27} + \frac{2b_3}{3} + c_2
$$

$$
v = -b_2 - \frac{a_2^2}{3}.
$$
Stability of the paramagnetic phase. In the paramagnetic phase \( w \propto q = 0 \), implying \( H_{\pm \pm} = 0 \), cf. equations (B.6)–(B.8) and the Hessian simplifies as \( H_2 = H_1 \). Its characteristic polynomial is

\[
P[H_2] = (\Lambda - \Lambda_4) \left( \Lambda - \frac{x}{2} \right) \left( -\Lambda^2 - b_2 \Lambda + c_2 \right)
\]  

where now, cf. equation (B.10):

\[
b_2 = \frac{3}{16} \left( \frac{2d^2 - 2d + 1}{(1-d)^2 d^2} - \beta^2 \delta_p^2 \right) 
\]  

\[
c_2 = \frac{1 - \beta^2 d^2 \delta_p^2}{32(1-d)^2 d^2}. 
\]  

Its zeros are

\[
\Lambda^{(2)}_1 = \frac{x}{2} \]  

\[
\Lambda^{(2)}_2 = \frac{-b_2 + \sqrt{b_2^2 - 4c_2}}{2} \]  

\[
\Lambda^{(2)}_3 = \frac{-b_2 - \sqrt{b_2^2 - 4c_2}}{2} \]  

\[
\Lambda^{(2)}_4 = \frac{1}{8} \left( \frac{1 - 2d + 2d^2}{d^2(1-d)^2} - \frac{p(p-1)\beta^2}{2} \right). 
\]

The first one is strictly positive for any \( p \).

The second one is always positive for \( p > 2 \) and ensures the stability of the PM solution in the whole phase space. For \( p = 2 \), instead, \( \Lambda^{PM}_4 \) marks the PM solution as unstable in the region where an SG solution exists and permits us to discard an unphysical solution, preventing a PM–PM first-order transition. \( \Lambda^{PM}_3 > \Lambda^{PM}_2 \) and, indeed, it is irrelevant.

The fourth eigenvalue, equal to the derivative of equation (33) with \( q = 0 \), allows us to discard another unphysical solution among the PM solutions.

Projection on subspace \( S_3 \)

In the subspace \( S_3 = (S_1 \cup S_2)^{\perp} \) \( (d(S_3) = 4) \) the Hessian reduces to a matrix \( H_3 = H_2 + O(n) \); indeed there are no new eigenvalues.

Appendix C. Stability of the 1RS solution

The paramagnetic solution is not affected by the ansatz choice; its stability analysis is indeed the same as the one in appendix B. Moreover for \( p = 2 \) is not necessary to break the replica symmetry, so in this section we choose \( p > 3 \) without loss of generality. These observations allow us to work directly with equations (32) and (33) imposed. Instead, in order to study also dynamical solution equation (34) is not imposed.
In the 1RSB ansatz the matrix (A.3) becomes

$$A_{ab}^{-1} = \frac{\delta_{ab}}{4\theta_0} - \frac{\eta_1 - \eta_0}{2m\theta_0\eta_0} \equiv x\delta_{ab} + w$$  \hspace{1cm} (C.1)

$$x \equiv \frac{1}{4\theta_0}$$  \hspace{1cm} (C.2)

$$w \equiv -\frac{\eta_1 - \eta_0}{2m\theta_0\eta_0}$$  \hspace{1cm} (C.3)

$$B_{a\neq b} = \frac{1}{32}\phi'(q_1)\epsilon_{ab} = \frac{\beta^2 p(p-1)}{64}q_1^{p-2}\epsilon_{ab} \equiv B_{q_1}\epsilon_{ab}$$  \hspace{1cm} (C.4)

$$B_{a=b} = \frac{\beta^2 p(p-1)}{64}q^{p-2} \equiv B_{d}$$  \hspace{1cm} (C.5)

where \(\epsilon_{ab}\) is the matrix introduced in section 3. For later convenience, it is useful to define

$$D_{\pm,\pm} \equiv \frac{x^2}{2}(\eta_0 \pm \theta)(\eta_0 \pm \theta)$$

$$E_{\pm,\pm} \equiv \frac{wx}{2}(\eta_0 \pm \theta)(\eta_0 \pm \theta) + \frac{m(xmw + x)(\eta_1 - \eta_0)(\eta_0 + (\pm 1 \pm 1/2)\theta + (\eta_1 - \eta_0)/4)}{2m}$$

$$G_{\pm,\pm} \equiv \frac{x^2(\eta_1 - \eta_0)^2}{4m^2} + \frac{wx(\eta_1 - \eta_0)((\pm 1 \pm 1/2)\theta + \eta_0 + (3/4)(\eta_1 - \eta_0))}{m}$$

and some linear combinations

$$E_{0}^{\pm,\pm} \equiv D_{\pm,\pm} + mE_{\pm,\pm} = \frac{x(x + mw)}{8}(\eta_1 + \eta_0 \pm 2\theta)(\eta_1 + \eta_0 \pm 2\theta)$$

$$G_{0}^{\pm,\pm} = D_{\pm,\pm} + 2mE_{\pm,\pm} + m^2G_{\pm,\pm} = \frac{(x + mw)^2}{2}(\eta_1 \pm \theta)(\eta_1 \pm \theta)$$

$$G_{1}^{\pm,\pm} = 2E_{\pm,\pm} + mG_{\pm,\pm}.$$

**Projection on subspace \(S_1\)**

\(S_{1,0}\). In the subspace \(S_{1,0}\), defined by

$$\delta r_{aa} = 0, \quad (\epsilon\delta q)_{ab} = (\delta q\epsilon)_{ab} = 0, \quad \delta q_{ab}\epsilon_{ab} = 0$$

with \(\text{dim}(S_{1,0}) = 3(n/2m^2)(n - m)(m^2 - 2m)\), the Hessian reduces to

$$H_{1,0} = \begin{pmatrix}
D_{++} & D_{+-} - \frac{x}{2} & -2D_{+-} \\
D_{+-} - \frac{x}{2} & D_{++} & -2D_{++} \\
-2D_{+-} & -2D_{+-} & 4D_{--} + x
\end{pmatrix}. \hspace{1cm} (C.7)
$$

Eigenvalues of \(H_{1,0}\):

$$\Lambda_{1,0}^{(1)} = \frac{x}{2}$$  \hspace{1cm} (C.8)

$$\Lambda_{1,0}^{(2,3)} = 2D_{--} + D_{++} + \frac{x}{4} \pm \sqrt{\left(2D_{--} - D_{++} + \frac{3x}{4}\right)^2 + 8D_{++}^2} \hspace{1cm} (C.9)$$

are always positive definite.

doi:10.1088/1742-5468/2011/12/P12005
Random, thermodynamic and inverse first-order transitions

$S_{1,1}$. In the subspace $S_{1,1}$, defined by

\[ \delta r_{aa} = 0, \quad (\epsilon \delta q)_{ab} = (\delta q \epsilon)_{ab} = 0, \quad \delta q_{ab}(1 - \epsilon_{ab}) = 0 \]

with $\dim(S_{1,1}) = 3(n/2)(m - 3)$:

\[
H_{1,1} \equiv \begin{pmatrix}
D_{++} - B_{q_1} & D_{++} - \frac{x}{2} - B_{q_1} & -2D_{+-} - 2B_{q_1} \\
D_{++} - \frac{x}{2} - B_{q_1} & D_{++} - B_{q_1} & -2D_{+-} - 2B_{q_1} \\
-2D_{+-} - 2B_{q_1} & -2D_{+-} - 2B_{q_1} & 4D_{--} + x - 4B_{q_1}
\end{pmatrix}
\]  

(C.10)

the eigenvalues are

\[
\Lambda_{1,1}^{(1)} = \frac{x}{2}
\]

(C.11)

\[
\Lambda_{1,1}^{(2,3)} = 2D_{--} + D_{++} + \frac{x}{4} - 3B_{q_1} \pm \sqrt{\left(2D_{--} - D_{++} + \frac{3x}{4} - B_{q_1}\right)^2 + 8(D_{+-} - B_{q_1})^2}.
\]

(C.12)

Since $\Lambda_{1,0}^{(1,2,3)}$ and $\Lambda_{1,1}^{(1)}$ are positive definite, the stability condition is expressed by $\Lambda_{1,1}^{(3)} > 0$, which reduces to

\[
\eta_1 > (p - 1)\eta_0
\]

(C.13)

which coincides with the dynamical condition, equation (39).

**Projection on subspace $S_2$**

$S_{2,0}$. In the subspace $S_{2,0}$, orthogonal to $S_{1,0} \cup S_{1,1}$ defined by

\[ \delta r_{aa} = 0, \quad (\epsilon \delta q \epsilon)_{ab} = 0, \quad (\delta q \epsilon)_{ab}\epsilon_{ab} = 0 \]

with $\dim(S_{2,0}) = 3(n/m)(n/m - 1)(m - 1)$, the Hessian reduces to

\[
H_{2,0} \equiv \begin{pmatrix}
E_{0}^{++} & E_{0}^{++} - 2x + mw & -2E_{0}^{+-} \\
E_{0}^{++} - 2x + mw & E_{0}^{++} & -2E_{0}^{+-} \\
-2E_{0}^{+-} & -2E_{0}^{+-} & 4E_{0}^{-} + 2x + mw
\end{pmatrix}.
\]

(C.14)

The characteristic polynomial is

\[
P[H_{2,0}] = \left(\Lambda - \frac{2x + mw}{4}\right) \left(\Lambda^2 - b_{20}\Lambda + c_{20}\right)
\]

(C.15)

with

\[
b_{20} = \frac{3[4\theta^2 + (1 + y)^2\eta_1^2]}{64y^2\theta^2\eta_1^2}
\]

\[
c_{20} = \frac{(1 + y)^2}{128y^2\theta^2\eta_1^2}
\]

with $y = \eta_0/\eta_1$, cf equation (36). The positiveness of both $b_{20}$ and $c_{20}$ implies positive zeros for the polynomial.

doi:10.1088/1742-5468/2011/12/P12005
In the subspace $S_{2,1}$, orthogonal to $S_{1,0} \cup S_{1,1}$ and restricted by

$$(\epsilon \delta r)_{ab} = \sum_{c} (\delta r_{ac} \epsilon_{ac}) = 0, \quad (\epsilon \delta q)_{ab} = 0, \quad (\delta q)_{ab}(1 - \epsilon_{ab}) = 0$$

(C.16)

with $\dim(S_{2,1}) = 3(n/m)(m - 1) + n - n/m$. Defining the matrix:

$$H'_{2,1} := \left( \begin{array}{cc} H_{1,1} & 0 \\ 0 & 4D_{-} + x - 4B_{n} \end{array} \right)$$

(C.17)

the Hessian projection in $S_{2,1}$ reduces to

$$H_{2,1} = H'_{2,1} + (m - 2) \left( \begin{array}{cccc} E_{++} & E_{+-} - \frac{y}{4} & -2E_{+}^{--} & -2E_{-}^{--} \\ E_{+-} - \frac{y}{4} & E_{++} & -2E_{+-} & -2E_{--} \\ -2E_{+}^{--} & -2E_{--} & 4E_{-}^{--} + \frac{y}{2} & 4E_{--}^{--} + \frac{y}{2} \\ -4E_{m}^{--} & -4E_{m}^{--} & 8E_{-}^{--} + \frac{y}{m} & 8E_{--}^{--} + \frac{y}{m} \end{array} \right).$$

(C.18)

This matrix has to be studied numerically on the static (and dynamic) 1RSB solution. In the whole $D,T$ plane it displays two real positive eigenvalues. The other two can be both real (and positive) or complex conjugated. In the region of $D,T$ values where complex eigenvalues occur they have a positive real part, apart from a small sub-region next to the static (resp. dynamic) RFOT transition line.

**Projection on subspace $S_{3}$**

In the subspace $S_{3,0}$, orthogonal to all other subspaces and defined by

$$\delta r_{aa} = 0, \quad (\epsilon \delta q \epsilon)_{ab}\epsilon_{ab} = 0$$

(C.19)

with $\dim(S_{3,0}) = 3(n/2m)(n/m - 1)$, the Hessian reduces to

$$H_{3,0} \equiv \left( \begin{array}{cccc} G_{0}^{++} & -\frac{x + mw}{2} & -2G_{0}^{--} \\ -\frac{x + mw}{2} & \frac{G_{0}^{++}}{2} & -2G_{0}^{+}^{+} \\ -2G_{0}^{--} & -2G_{0}^{+}^{+} & 4G_{0}^{--} + 2x + mw \end{array} \right).$$

(C.20)

The characteristic polynomial is

$$P[H_{3,0}] = \left( \Lambda - \frac{2x + mw}{4} \right) (\Lambda^{2} - b_{30}\Lambda + c_{30})$$

(C.21)

with

$$b_{30} = \frac{3}{16} \left( \frac{1}{\theta^{2}} + \frac{1}{\eta_{1}^{2}} \right)$$

and

$$c_{30} = \frac{1}{32(\theta^{2}\eta_{1}^{2})}$$

the positiveness of both $b_{30}$ and $c_{30}$ implies positive zeros for the polynomial.
$S_{3,1}$. In the subspace $S_{3,1}$, orthogonal to all other subspaces and restricted by

$$(\epsilon \delta q \epsilon)_{ab}(1 - \epsilon_{ab}) = 0 \quad (C.22)$$

with $\dim(S_{3,1}) = 4(n/m)$ the Hessian reduces to

$$H_{3,1} = H'_{2,1} + (m - 1) \begin{pmatrix}
G_{1}^{++} & G_{1}^{++} - \frac{y}{2} & -2G_{1}^{+-} & -2G_{1}^{--} \\
G_{1}^{+-} - \frac{y}{2} & G_{1}^{++} & -2G_{1}^{-+} & -2G_{1}^{--} \\
-2G_{1}^{+-} & -2G_{1}^{--} & 4G_{1}^{-+} + y & 4G_{1}^{--} + y \\
-4G_{m-1}^{+-} & -4G_{m-1}^{--} & \frac{8G_{m-1}^{-+} + y}{m-1} & \frac{8G_{m-1}^{--} + y}{m-1}
\end{pmatrix}. \quad (C.23)$$

Also this matrix has to be studied numerically as equation (C.18) and we evaluated its values point by point in the phase diagram. This matrix, as well, has two real positive definite eigenvalues together with two complex conjugated eigenvalues (in a region of the $D,T$ plane). Some points, next to the RFOT transition, have complex eigenvalues with negative real part. Comparing with the study of compressibility, cf section 5.4.1, all points with a negative compressibility also have at least two complex eigenvalues with a negative real part. The opposite, as we have shown in figure C.1, is not always true.

References

[1] Rastogi S, Höhne G W H and Keller A, 1999 Macromolecules 32 8897
Greer A L, 2000 Nature 404 134
van Ruth N J L and Rastogi S, 2004 Macromolecules 37 8191

[2] Plazanet M et al, 2004 J. Chem. Phys. 121 5031
Tombari E et al, 2005 J. Chem. Phys. 123 054104
Plazanet M et al, 2006 J. Chem. Phys. 125 154504
Plazanet M et al, 2006 Chem. Phys. 331 35
Angelini R and Ruocco G, 2007 Phil. Mag. 87 553
Ferrari C et al, 2007 J. Chem. Phys. 126 124506
Angelini R, Salvi G and Ruocco G, 2008 Phil. Mag. 88 4109
Angelini R, Ruocco G and De Panfilis S, 2008 Phys. Rev. E 78 020502
Plazanet M, Johnson M R and Trommsdorff H P, 2009 Phys. Rev. E 79 053501
Angelini R, Ruocco G and De Panfilis S, 2009 Phys. Rev. E 79 053502

[3] Haque A and Morris E R, 1993 Carb. Pol. 22 161
Chevillard C and Axelos M A V, 1997 Colloid Polym. Sci. 275 537
Random, thermodynamic and inverse first-order transitions

Hirrien M et al, 1998 Polymer 39 6251
[4] Blume M, Emery V J and Griffiths R B, 1971 Phys. Rev. A 4 1071
[5] Capel H W, 1966 Physica 32 966
Blume M, 1966 Phys. Rev. 141 517
[6] Schupper N and Shnerb N M, 2004 Phys. Rev. Lett. 93 037202
[7] Schupper N and Shnerb N M, 2005 Phys. Rev. E 72 046107
[8] Ghatak S K and Sherrington D, 1977 J. Phys. C: Solid State Phys. 10 3149
[9] Lages E J S and de Almeida J R L, 1982 J. Phys.: Solid State Phys. C 15 L1187
[10] Mottishaw P J and Sherrington D, 1985 J. Phys.: Solid State Phys. C 18 5201
[11] da Costa F A, Yokoi C S O and Salinas R A, 1994 J. Phys. A: Math. Gen. 27 3365
[12] Arenzon J J, Nicodemi M and Sellitto M, 1996 J. Physique I 6 1143
[13] Sellitto M, Nicodemi M and Arenzon J J, 1997 J. Physique I 7 945
[14] da Costa F A, Nobre F D and Yokoi C S O, 1997 J. Phys. A: Math. Gen. 30 2317
[15] Schreiber G R, 1999 Eur. Phys. J. B 9 479
[16] da Costa F A and de Araujo J M, 2000 Eur. Phys. J. B 15 313
[17] Albino A Jr, Nobre F D and da Costa F A, 2000 J. Phys.: Condens. Matter 12 5713
[18] Crisanti A and Leuzzi L, 2002 Phys. Rev. Lett. 89 237204
[19] Crisanti A and Leuzzi L, 2004 Phys. Rev. B 70 014409
[20] Crisanti A and Leuzzi L, 2005 Phys. Rev. Lett. 95 087201
[21] da Costa F A, 2010 Phys. Rev. B 82 052402
[22] Parisi G, 1979 Phys. Lett. A 73 203
[23] Parisi G, 1980 J. Phys. A: Math. Gen. 13 L115
[24] M´ezard M, Parisi G and Virasoro M, 1987 Spin Glass Theory and Beyond (Singapore: World Scientific)
[25] Paoluzzi M, Leuzzi L and Crisanti A, 2010 Phys. Rev. Lett. 104 120602
[26] Leuzzi L, Paoluzzi M and Crisanti A, 2011 Phys. Rev. B 83 014107
[27] Ozelik V O and Berker A N, 2008 Phys. Rev. E 78 031104
[28] Antenucci F, Crisanti A and Leuzzi L, in preparation
[29] Kirkpatrick T R and Thirumalai D, 1987 Phys. Rev. Lett. 58 2091
[30] Bray A J and Moore M A, 1981 J. Phys. A: Math. Gen. 14 L377
[31] Crisanti A and Sommers H-J, 1992 Z. Phys. B 87 341
[32] Crisanti A, Leuzzi L and Rizzo T, 2003 Eur. Phys. J. B 36 129
[33] Cavagna A, 2009 Phys. Rep. 476 51
[34] Sciortino F, 2005 J. Stat. Mech. P05015
[35] Binder K and Kob W, 2005 Glassy Materials and Disordered Solids (Singapore: World Scientific)
[36] Leuzzi L and Nieuwenhuizen T M, 2007 Thermodynamics of the Glassy State (London: Taylor and Francis)
[37] Götze W, 2009 Complex Dynamics of Glass-Forming Liquids: A Mode-Coupling Theory (Oxford: Oxford University Press)
[38] Gibbs J H and Di marzio E A, 1958 J. Chem. Phys. 28 373
[39] Marinari E, Parisi G and Ritort F, 1994 J. Phys. A: Math. Gen. 27 7615
[40] Marinari E, Parisi G and Ritort F, 1994 J. Phys. A: Math. Gen. 27 7647
[41] Sellitto M, 2006 Phys. Rev. B 73 180202
[42] Gross D J, Kanter I and Sompolinsky H, 1985 Phys. Rev. Lett. 55 304
[43] Gardner E, 1985 Nucl. Phys. B 257 747
[44] Mottishaw P J, 1986 Europhys. Lett. 1 409
[45] Griffiths R B, 1967 Physica 33 689
[46] Caiazzo A, Coniglio A and Nicodemi M, 2002 Phys. Rev. E 66 046101
[47] Caiazzo A, Coniglio A and Nicodemi M, 2004 Phys. Rev. Lett. 93 215701
[48] Caiazzo A, Coniglio A and Nicodemi M, 2004 Europhys. Lett. 65 256–61
[49] Kosterlitz J M, Thouless D J and Jones R C, 1976 Phys. Rev. Lett. 36 1217

doi:10.1088/1742-5468/2011/12/P12005