

Metastable states and space-time phase transitions in a spin-glass modelRobert L. Jack¹ and Juan P. Garrahan²¹*Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom*²*School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom*

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We study large deviations of the dynamical activity in the random orthogonal model. This is a fully connected spin-glass model with one-step replica symmetry-breaking behavior, consistent with the random first-order transition scenario for structural glasses. We show that this model displays dynamical (space-time) phase transitions between active and inactive phases, as demonstrated by singularities in large deviation functions. We argue that such transitions are generic in systems with long-lived metastable states.

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I. INTRODUCTION

Glass transitions and glassy dynamics occur in a wide range of systems, including structural glasses [1], colloidal suspensions, granular media [2], and spin glasses [3]. As their glass transitions are approached, the relaxation in these systems slows down dramatically but their structure remains disordered. The increasing relaxation time is often assumed to be a consequence of an underlying (continuous) phase transition [4–6], but the existence of such a transition in structural glasses remains unproven.

We and others have recently proposed that even if no thermodynamic phase transition exists in glass formers, the underlying transition might be a (discontinuous) “space-time” phase transition [7–9], occurring in trajectory space. By applying a thermodynamic (large deviation) formalism to ensembles of trajectories [10,11], one constructs dynamical free energies, whose singularities can be interpreted as dynamical phase transitions. The existence of such first-order transitions can be proven in idealised lattice models, known as kinetically constrained models (KCMs) [8]. Furthermore, computer simulations reveal behavior consistent with these phase transitions in atomistic model glass formers [9]. Physically, the idea [7] is that the characteristic features of glassy systems arise from coexistence between active and inactive dynamical phases.

Here, we consider the random orthogonal model (ROM) [12,13], a fully connected spin-glass model that realizes the one-step replica symmetry-breaking (1-RSB) scenario. This scenario is the basis for a mean-field theory of structural glasses, the random first-order transition theory [5]. We show that the ROM supports coexisting dynamical phases, separated by first-order space-time phase transitions, as in KCMs.

This similarity is surprising, since KCMs and the ROM are motivated by quite different assumptions about the behavior of supercooled liquids and glassy materials. In KCMs, slow dynamics arise from the tendency of particles to obstruct each other, so that motion is impossible in almost all regions of the system, except for a few mobile regions where particles can move. Such an approach is naturally associated with very heterogeneous dynamics [14,15], and observations of dynamical heterogeneity in glassy systems [16] have often been used to motivate studies of KCMs. On the other hand, in 1-RSB systems, one begins from a homogeneous (mean-

field) approach, associating glassy behavior with a large number of metastable states, with rare transitions between them (see [17] for a recent review of some of the relevant ideas). Such transitions involve the system behaving in a cooperative manner in order to cross large (free-)energy barriers. Such models still support dynamical heterogeneity, but the nature of the associated fluctuations seems quite different.

Nevertheless, despite these significant differences, both KCMs and the ROM are united by the presence of very long-lived (metastable) states: we argue that the space-time thermodynamic formalism reveals the presence of such states, both through analytic calculations and computer simulations. Our analysis of metastable states is closely related to previous work, such as that of Biroli and Kurchan [18]. The large deviation method we use, however, not only leads to important physical insight, but allows investigation of these ideas numerically in realistic models [7–9]. The work presented in the following sections shows that these methods can be used to reveal the presence of metastable states in 1-RSB models, highlighting their general applicability in glassy systems.

II. FORMALISM AND MODEL DEFINITION

Our approach is to apply thermodynamic methods to measures of dynamical activity, as described in [8]. Consider a system of N spins (or N particles), evolving with stochastic dynamics, at temperature T . We define

$$Z(s, t_{\text{obs}}) = \langle e^{-sK} \rangle_0, \quad (1)$$

where K is a measure of activity and the average is taken over trajectories that run from an initial time $t=0$ to a final time $t=t_{\text{obs}}$, in an equilibrated system. (Such averages are denoted by $\langle \cdot \rangle_0$.) In the ROM, the configuration space is discrete and we take K to be the number of changes of configuration (kinks), or dynamical activity in the trajectory [7,19,20]. For large t_{obs} , then

$$Z(s, t_{\text{obs}}) \sim e^{t_{\text{obs}}\psi(s)}. \quad (2)$$

Here, the function $\psi(s)$ is a large deviation function, and can be thought of as a “space-time” free energy. Its singularities are space-time phase transitions: i.e., qualitative changes in

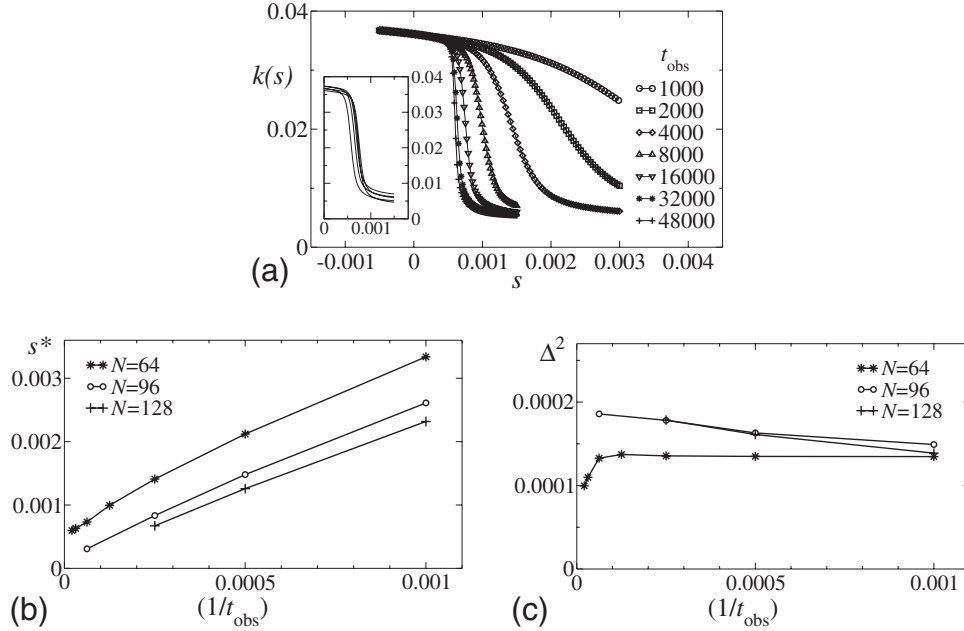


FIG. 1. Space-time phase transition in the ROM. (a) Average activity $k(s)$ as a function of s for $N=64$ and fixed disorder at $T=1/5 > T_d$. The equilibrium relaxation time at this temperature is $\tau \approx 110$ (in units of MC sweeps). The crossover in $k(s)$ becomes increasingly sharp as t_{obs} increases. The inset to (a) shows $k(s)$ for five different disorder realizations for $t_{\text{obs}}=16\,000$. (b) Dependence of s^* on observation time and system size. (c) Dependence of $\Delta^2 = \chi^*/(Nt_{\text{obs}})$ on the system size. As discussed in the text, the scaling in panels (b) and (c) is compatible with a space-time phase transition at $s=0$.

ensembles of trajectories. Interpreting $Z(s, t_{\text{obs}})$ as the partition function for a biased ensemble of trajectories (the “ s ensemble”), we define expectation values within this ensemble as

$$\langle A \rangle_s = \frac{1}{Z(s, t_{\text{obs}})} \langle A e^{-sK} \rangle_0. \quad (3)$$

In particular,

$$k(s) \equiv \frac{1}{Nt_{\text{obs}}} \langle K \rangle_s \quad (4)$$

is the mean activity in the s -ensemble. In the limit of large t_{obs} then $k(s) \rightarrow -\frac{1}{N} \psi'(s)$. (The ensemble with $s=0$ is simply the equilibrium ensemble of trajectories.)

The ROM [12] consists of N Ising spins $\sigma_i = \pm 1$ ($i = 1, \dots, N$) and an energy function $E = 1/2 \sum_{i \neq j} J_{ij} \sigma_i \sigma_j$. The matrix of quenched random couplings J_{ij} is symmetric and orthogonal. We construct it as $J = R^T D R$ where $D = \text{diag}(1, -1, 1, -1, \dots)$ and R is a randomly generated $O(N)$ rotation. Consistent with the 1-RSB scenario in the $N \rightarrow \infty$ limit, there are three important temperatures for the ROM [12]: the static transition temperature $T_K = 0.065$ below which replica symmetry is broken; the dynamical transition temperature $T_d = 0.134$ below which the equilibrium correlation function has a nonzero limit as $t \rightarrow \infty$; and the onset temperature $T_o = 0.32$ below which long-lived Thouless-Anderson-Palmer (TAP) states exist [18, 21, 22].

The ROM is straightforwardly simulated using Monte Carlo dynamics. Time is measured in Monte Carlo sweeps throughout, and the only parameter of the model is the temperature T . We focus first on the regime $T_d < T < T_o$ which is

the most relevant one for supercooled liquids. We use transition path sampling [23] to sample the s ensemble, as described in [9]. We show results for $N \geq 64$ and for representative realizations of the disorder J_{ij} . Our results depend weakly on the realization of the disorder, but we have not analyzed sample-to-sample fluctuations in detail due to the computational effort associated with sampling the s -ensemble (see [13] for an analysis at equilibrium).

III. RESULTS

A. “Supercooled” regime, $T_d < T < T_o$

Figure 1(a) shows the mean activity $k(s)$ in the s -ensemble at temperature $T=1/5$. Clearly, $k(s)$ decreases sharply as s is increased from zero. That is, there is a crossover from active behavior for $s \leq 0$ to inactive behavior for larger s , and this crossover becomes increasingly sharp as N and t_{obs} are increased. The inset to Fig. 1(a) suggests that this crossover is independent of the precise realization of the disorder J_{ij} . The susceptibility

$$\chi(s) \equiv k'(s) \quad (5)$$

peaks at the inflection point of the curves in panel (a). Let s^* be the value of s that maximizes χ , and let $\chi^* \equiv \chi(s^*)$ be the maximal susceptibility. Figure 1(b) shows that s^* decreases toward zero with increasing N and t_{obs} . We also define

$$\Delta^2 = \frac{\chi^*}{Nt_{\text{obs}}} \quad (6)$$

which is equal to the maximal variance in the (intensive) activity $k(s)$. In the absence of phase transitions, one expects

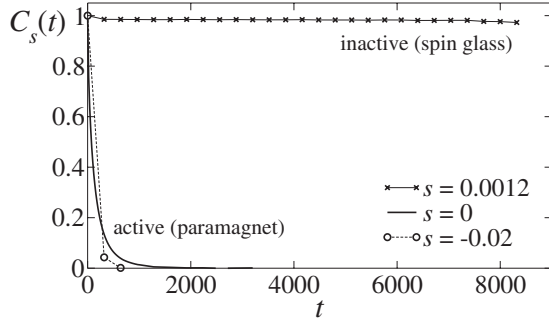


FIG. 2. Dynamics in active and inactive phases. Autocorrelation functions $C_s(t)$ in the ROM at $T=1/5$, for $N=64$ and $t_{\text{obs}}=16000$, illustrating active and inactive phases obtained by varying s .

$\Delta^2 \rightarrow 0$ if one takes large enough N and t_{obs} . (By analogy with thermodynamics, the variance of intensive quantities vanishes as the system size is taken to infinity, as long as the free-energy density $\frac{1}{N}\psi(s)$ exists and remains analytic in the limit of large N .) However, Fig. 1(c) shows that Δ^2 tends to a finite limiting value when the space-time volume $N \times t_{\text{obs}}$ gets large enough [24]. The finite-size scaling of Figs. 1(b) and 1(c) is consistent with a sharp (first-order) transition at $s^*=0$. We interpret $s=0$ as a line of “dynamical phase coexistence” [8].

The dependence of s^* on N and t_{obs} limits the accuracy of our finite-size scaling analysis. The reason for this effect is that the s -ensemble is time-translational invariant (TTI) only for times $0 \leq t \leq t_{\text{obs}}$, with deviations from TTI behavior [8] near the initial and final times. These boundary effects enhance the contribution of the active phase to $Z(s, t_{\text{obs}})$, so that for fixed N we expect that $s^* = s_N + O(1/t_{\text{obs}})$, consistent with Fig. 1(b). The scaling of χ^* and s^* with N can be accounted for by considering the lifetimes of metastable (TAP) states in finite systems. Briefly, if N is finite then all metastable states have finite lifetimes and $\psi(s)$ is analytic for all s [24].

We characterize the dynamical behavior of the ROM in the s ensemble via the autocorrelation function,

$$C_s(t) = \frac{1}{N} \left\langle \sum_i \sigma_i(t'+t) \sigma_i(t') \right\rangle_s, \quad (7)$$

which is independent of t' for $0 \leq t' < t+t' \leq t_{\text{obs}}$ [8]. Figure 2 shows this function for values of s on both sides of the dynamical transition. We have $T > T_d$, so the equilibrium dynamics of the ROM are ergodic, and $C_{s=0}(t)$ decays to zero with a finite relaxation time τ . For $s < 0$, states with high activity dominate the s -ensemble and the trajectories resemble those at equilibrium. However, for $s > 0$, states with low activity predominate, and Fig. 2 shows that $C_s(t)$ remains finite on the longest time scales that we can sample. We define $q_{\text{EA}} \equiv \lim_{t \rightarrow \infty} C_s(t)$, with the limit taken after the limits of large N and t_{obs} .

B. Generic 1-RSB systems in the s ensemble

We now show that systems realizing the 1-RSB scenario have a first-order dynamical transition from a “paramagnetic state” with $q_{\text{EA}}=0$ to a “spin glass” with finite q_{EA} , as s is

increased through zero. This is consistent with Figs. 1 and 2 since the ROM realizes this scenario.

Our discussion rests on the existence of a large number of metastable states, which can be studied within the TAP approach [18,21,22]. The presence of TAP states is sufficient to prove the existence of a space-time phase transition. Let \mathbb{W} be the master operator associated with the stochastic dynamics of the system, as in [8]. Consistent with the 1-RSB scenario, we assume a separation of time scales, corresponding to conditions on the eigenspectrum of \mathbb{W} : There is a spectrum of fast rates larger than some cutoff γ_f and a spectrum of slow rates smaller than a second cutoff $\gamma_s \ll \gamma_f$. On starting in a given configuration, the system relaxes quickly into a metastable (TAP) state in a time of order γ_f^{-1} . However, transitions between these states occur much more slowly, taking a time of order γ_s^{-1} . Then, for $\gamma_f^{-1} \ll t_{\text{obs}} \ll \gamma_s^{-1}$, the time evolution operator of the system is a projection operator onto the TAP states,

$$e^{\mathbb{W}t_{\text{obs}}} = \sum_{\alpha} |P_{\alpha}\rangle \langle Q_{\alpha}| + O(e^{-\gamma_f t_{\text{obs}}}) + O(\gamma_s t_{\text{obs}}), \quad (8)$$

where $|P_{\alpha}\rangle$ describes the (metastable) equilibrium distribution within state α , and $\langle Q_{\alpha}|$ gives the probabilities of relaxation into state α [25]. This result was used in [18], where the trace of $e^{\mathbb{W}t}$ was used to estimate the number of metastable states with lifetimes greater than t^* .

Now, the partition sum $Z(s, t_{\text{obs}})$ has a transfer-matrix representation and the free energy $\psi(s)$ is the largest eigenvalue of a transfer operator $\mathbb{W}(s)$ [19,26], whose matrix elements are

$$\langle C' | \mathbb{W}(s) | C \rangle = \begin{cases} \langle C' | \mathbb{W} | C \rangle e^{-s}, & C \neq C' \\ \langle C' | \mathbb{W} | C \rangle, & C = C' \end{cases}, \quad (9)$$

where $|C\rangle$ is a ket representing a single configuration of the system. Clearly, $\mathbb{W}(0) = \mathbb{W}$. Alternatively, one may write

$$\mathbb{W}(s) = e^{-s} \mathbb{W} + (e^{-s} - 1) \mathbb{R}, \quad (10)$$

where \mathbb{R} is a diagonal operator whose elements are the escape rates from the configurations of the system $\langle C | \mathbb{R} | C' \rangle = -\langle C | \mathbb{W} | C \rangle \delta_{C,C'}$.

Since the stochastic dynamics of the ROM obey detailed balance, $\mathbb{W}(s)$ may be symmetrized, and its largest eigenvalue can be estimated variationally [8] so that

$$\psi(s) \geq \frac{\langle \Psi | e^{\hat{E}T} \mathbb{W}(s) | \Psi \rangle}{\langle \Psi | e^{\hat{E}T} | \Psi \rangle} \quad (11)$$

for any trial state $|\Psi\rangle$, with equality when $|\Psi\rangle$ is the right eigenvector of $\mathbb{W}(s)$ with largest eigenvalue. Here, \hat{E} is the energy operator of the system, and we take $k_B=1$.

For $s \ll 1$ and $\gamma_s \ll \gamma_f$, we take the variational ansatz $|\Psi\rangle = |P_{\alpha}\rangle$, and vary α . In the remainder of this section, we take γ_f as the fundamental unit of time, which keeps our notation compact. For example, we can write

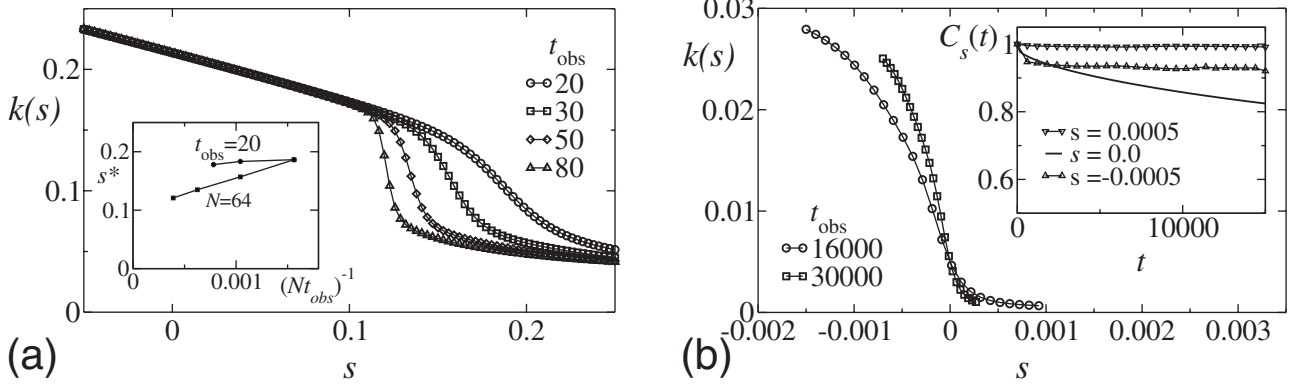


FIG. 3. Transitions in the ROM for $T > T_0$ and $T < T_d$. (a) Mean activity $k(s)$ as a function of s at $T = 1/2 > T_0$ for increasing t_{obs} at $N = 64$ and fixed disorder (cf. Fig. 1). The equilibrium correlation time at this temperature is $\tau \approx 4$. Inset: effect on s^* of increasing N and t_{obs} . These observations are consistent with a transition at finite s^* in the thermodynamic limit. [On increasing t_{obs} at $N = 64$, $\chi^*/(Nt_{\text{obs}})$ increases weakly (not shown).] (b) Mean activity $k(s)$ at $T = 1/9 < T_d$ for $N = 64$. The behavior of $k(s)$ is consistent with a first-order transition at $s^* = 0$. Inset: autocorrelation $C_s(t)$ for $t_{\text{obs}} = 3 \times 10^4$ for various s . The relaxation time at $s = 0$ is $\tau \approx 10^7$, although this depends strongly on system size since $T < T_d$.

$$\psi(s) \geq \psi_{\text{var}}(s) = -N \min_{\alpha} [s k_{\alpha}] + O(\gamma_s) + O(s^2), \quad (12)$$

where $k_{\alpha} \equiv N^{-1} \langle Q_{\alpha} | R | P_{\alpha} \rangle$ is the average value of the activity density $K/(Nt_{\text{obs}})$ for trajectories at (metastable) equilibrium in state α . [Strictly, we are expanding $\psi(s)/\gamma_f$ over both s and γ_s/γ_f . We also used $\langle Q_{\alpha} | = \langle P_{\alpha} | e^{\tilde{E}/T} + O(\gamma_s)$ [18,25] and the fact that the $|P_{\alpha}\rangle$ are nonzero only in nonoverlapping regions of configuration space.] For $(\gamma_s/\gamma_f) \ll |s| \ll 1$, we will show that the bound is saturated, and

$$k(s) \approx \theta(s) \min_{\alpha} [k_{\alpha}] + \theta(-s) \max_{\alpha} [k_{\alpha}], \quad (13)$$

where $\theta(s)$ is the step function.

To demonstrate saturation of the bound, we use the representation of Eq. (10), and consider the operator $e^s \mathbb{W}(s)$, for which the field s only appears in diagonal matrix elements. If one then transforms to a basis consisting of the $|P_{\alpha}\rangle$ and $\langle Q_{\alpha}|$, together with the fast eigenvectors of \mathbb{W} , the original assumptions on the spectrum of \mathbb{W} imply that

$$e^s \mathbb{W}(s) = \sum_{\alpha} |P_{\alpha}\rangle \phi_{\alpha} \langle Q_{\alpha}| + e^s \sum_{\alpha, \beta \neq \alpha} |P_{\alpha}\rangle h_{\alpha\beta} \langle Q_{\beta}| + e^s \mathbb{W}^{\text{fast}}(s), \quad (14)$$

where $\phi_{\alpha} = -k_{\alpha} s + O(s^2) + O(\gamma_s)$, the $h_{\alpha\beta} = O(\gamma_s)$ are the (slow) transition rates between the metastable states, and all eigenvectors of $\mathbb{W}^{\text{fast}}(s)$ are greater than $\gamma_f + O(s)$. (We used the fact that $\langle Q_{\alpha} | P_{\beta} \rangle = \delta_{\alpha\beta} + O(\gamma_s)$ [18,25].) In this case, using a linear combination of the $|P_{\alpha}\rangle$ as an ansatz for $|\Psi\rangle$ improves on the variational bound of Eq. (12) by at most $O(\gamma_s)$, while a combination of the $|P_{\alpha}\rangle$ with the fast eigenvectors of \mathbb{W} gives an improvement that is $O(s^2)$. Thus, Eq. (12) holds as an equality.

In the 1-RSB scenario, the slow rate γ_s vanishes in the limit of large N . Taking this limit, followed by a limit of large t_{obs} , Eq. (13) holds as $|s| \rightarrow 0$. Hence, if the states α cover a finite range of k_{α} then $k(s)$ is discontinuous at $s = 0$. Thus, if γ_f is finite and $\gamma_s \rightarrow 0$, there is a first-order dynamical transition at $s = 0$, similar to that seen in KCMs [8]. The

prediction of Eq. (13) and the numerical observations of Figs. 1 and 2 constitute the key results of this paper: for $T_d < T < T_0$, the ROM has a first-order space-time phase transition at $s = 0$.

In thermodynamics, first-order phase transitions are characterized by singular responses to boundary fields. We take $s = 0$ and $T_d < T < T_0$, and consider an ensemble of trajectories with initial conditions that are equilibrated at temperature T' . Within the 1-RSB scenario, the system relaxes into the equilibrium (active) state for $T' > T_d$, but for $T' < T_d$ it relaxes into a metastable state with finite q_{EA} [22]. In the language of the s -ensemble, the temperature T' corresponds to a boundary field on the trajectories, and the singular response at $T' = T_d$ may be linked with wetting phenomena [9,27].

C. High temperatures, $T > T_0$

So far we have considered only $T_d < T < T_0$. For temperatures above the onset temperature, $T > T_0$, metastable states are no longer infinitely long-lived and the slow rate γ_s remains finite even as $N \rightarrow \infty$. It follows that $k(s)$ is continuous at $s = 0$. In the absence of a diverging slow time scale associated with the operator \mathbb{W} , one might expect $k(s)$ to be analytic for all s . However, for $T > T_0$, analytic arguments and numerical results both indicate a first-order dynamic phase transition between active and inactive phases that occurs at $s^* > 0$. Figure 3(a) shows the numerical evidence for this transition. Dynamical phase transitions at finite s have been found in other spin models for which all states have finite lifetimes [19,28].

For the analytic argument in favor of this scenario, consider the proposed phase diagram shown in Fig. 4, where we show the boundary between active and inactive phases occurring at $s^* > 0$ for $T > T_0$. An alternative scenario would be for the first-order line to end at a critical point at $(s_c, T_c) = (0, T_0)$. However, we reject this for two reasons: first, we have $q_{\text{EA}} = 0$ for large T and small $s > 0$, while $q_{\text{EA}} > 0$ for low T and small $s > 0$. Standard arguments based on conti-

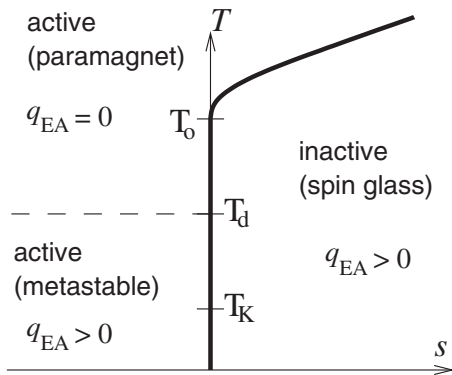


FIG. 4. Proposed space-time phase diagram. The heavy line is a first-order transition between active and inactive dynamical phases. We expect dynamical phase coexistence at $s=0$ in 1-RSB systems for all temperatures below the onset temperature T_0 . For $T > T_0$ coexistence takes place at $s > 0$. The dashed line separates the metastable active state of Fig. 3(b) from the paramagnetic active state of Fig. 1.

nuity of the free energy indicate that these two qualitatively different regimes must be separated by some kind of phase transition. (For similar reasons, no critical point is possible for liquid/crystal phase boundaries.) Second, a critical point at $(s_s, T_c) = (0, T_0)$ should be accompanied by diverging fluctuations at this point, and no such divergence is observed in the well-characterized equilibrium behavior as $T \rightarrow T_0^+$ for $s = 0$. Combining these arguments with the numerical results of Fig. 3, we prefer the scenario shown in Fig. 4 to any kind of critical point near T_0 .

D. Low temperatures $T < T_d$

Finally, we consider the behavior of the system for $T < T_d$. In this regime, 1-RSB systems have “threshold” states which are associated with aging behavior [29]. The relaxation time within the paramagnetic state diverges, and the “gap” ($\gamma_f - \gamma_s$) vanishes. This complicates the analysis of the transition at $s=0$.

We may evaluate the bound in Eq. (12), although we exclude the paramagnetic state from the minimization. As long as the minimization contains states with a finite range of k_α , Eq. (12) establishes the existence of a first-order space-time phase transition for $T < T_d$, similar to that for $T > T_d$. Figure 3(b) shows numerical results consistent with such a transition. However, in the absence of a gap, one may no longer prove that bound (12) is saturated, so one may not identify

the states at small positive and small negative s with single metastable states α that extremize k_α . Nevertheless, the numerical results show that q_{EA} remains finite for $s < 0$, suggesting that the active state is constructed from active metastable states and not from paramagnetic “threshold” states.

E. Proposed phase diagram

The dynamical phase structure of the ROM is summarized in the (s, T) phase diagram of Fig. 4. For temperatures between the dynamical transition temperature and the onset of metastability, $T_d < T < T_0$, metastable states lead to a first-order dynamical phase transition at $s=0$ (Fig. 1). Thus, the equilibrium ensemble of trajectories is associated with coexistence between active (ergodic) and inactive phases. Above T_0 , all metastable states in the model have finite lifetimes, and the coexistence line moves to finite s [Fig. 3(a)]. For $T < T_d$, the first-order transition remains at $s=0$ but it now separates dynamics within metastable states with high and low activity [Fig. 3(b)]. This suggests that for $s < 0$ there is a transition near T_d between an active ergodic phase with $q_{EA}=0$ and an active but nonergodic phase in which the activity $k(s)$ is larger than its equilibrium value $k(0)$ but $q_{EA} > 0$ [28]. At T_K the system undergoes an “entropy crisis:” for $T < T_K$, the TAP states are numerous although their associated entropy (complexity) vanishes. Nevertheless, our arguments for $T < T_d$ still apply, indicating that the transition remains at $s=0$.

We have focused on the ROM in this paper, but Eqs. (12) and (13) indicate that phase diagrams for generic 1-RSB systems should be similar to Fig. 4. How this picture differs between mean-field and finite-dimensional systems is an important open question. Our main conclusion is that dynamical phase coexistence between active and inactive phases is not restricted to idealized KCMs [8] but also present in atomistic liquids [9], and, as we have shown here, in spin glasses. We conclude that the s ensemble is the natural method for studying inactive and metastable states and their consequences in glassy systems in general.

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