Metastable states and space-time phase transitions in a spin-glass model

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We study large deviations of the dynamical activity in the random orthogonal model (ROM). This is a fully connected spin-glass model with one-step replica symmetry breaking behaviour, 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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Glass transitions and glassy dynamics occur in a wide range of systems, including structural glasses\textsuperscript{[1]}, colloidal suspensions, granular media\textsuperscript{[2]} and spin glasses\textsuperscript{[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\textsuperscript{[4,5]}, 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\textsuperscript{[6,7]}, occurring in trajectory space. By applying a thermodynamic (large deviation) formalism to ensembles of trajectories\textsuperscript{[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)\textsuperscript{[8]}. Furthermore, computer simulations reveal behaviour consistent with these phase transitions in atomistic model glass-formers\textsuperscript{[9]}. Physically, the idea\textsuperscript{[12]} 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)\textsuperscript{[12,13]}, a fully-connected spin-glass model that realises the one-step replica symmetry breaking (1-RSB) theory\textsuperscript{[2]}. Physically, the idea\textsuperscript{[2]} 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)\textsuperscript{[12,13]}, a fully-connected spin-glass model that realises 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\textsuperscript{[2]}. We show that the ROM supports coexisting dynamical phases, separated by first-order space-time phase transitions, as in KCMs. We argue that these transitions occur in systems with long-lived metastable states, including generic 1-RSB models.

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

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

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. In the ROM, the configuration space is discrete and we take $K$ to be the number of changes of configuration (kinks) in the trajectory\textsuperscript{[14,15]}. For large $t_{\text{obs}}$, then $Z(s, t_{\text{obs}}) \sim e^{t_{\text{obs}}} \psi(s)$. 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 ensembles of trajec-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{\textbf{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 $t_{\text{obs}}$ increases. The inset to (a) shows $k(s)$ for five different disorder realisations for $t_{\text{obs}} = 16000$. (b) Dependence of $s^*$ and $\chi^*$ (inset) on observation time and system size. This scaling compatible with a space-time phase transition at $s = 0$.}
\end{figure}
is the mean activity in the large $t = 64$ and tocorrelation functions
Dynamics in active and inactive phases
phases obtained by varying $J$ dominates couplings $J_i$, $s \equiv \langle s \rangle = 1$ is symmetric and orthogonal. We construct it as $J = R^T DR$ where $D = \text{diag}(1, -1, 1, -1, \ldots)$ and $R$ is a randomly generated $O(N)$ rotation. Consistent with the 1-RSB scenario in the $N \to \infty$ limit, there are three important temperatures for the ROM: 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 non-zero limit as $t \to \infty$; and the onset temperature $T_o = 0.32$ below which long-lived Thouless-Anderson-Palmer (TAP) states exist.

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 [18] to sample the $s$-ensemble, as described in [8]. We show results for $N \geq 64$ and for representative realisations of the disorder $J_{ij}$. Our results depend weakly on the realisation of the disorder, but we have not analysed sample-to-sample fluctuations in detail due the computational effort associated with sampling the $s$-ensemble (see [13] for an analysis at equilibrium).

Fig. 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 behaviour for $s \leq 0$ to inactive behaviour 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 realisation of the disorder $J_{ij}$. The susceptibility $\chi(s) \equiv k^2(s)$ peaks at the inflection point of the curves in panel (a). Let $s^*$ be the value of $s$ that maximises $\chi$, and let $\chi^* \equiv \chi(s^*)$ be the maximal susceptibility. Fig. 1(b) shows that $s^*$ decreases towards zero with increasing $N$ and $t_{obs}$, and $\chi^*$ diverges linearly with the space-time volume $N \times t_{obs}$. This finite size scaling is consistent with a sharp (first-order) transition at $s^* = 0$. We interpret $s = 0$ as a line of ‘dynamical phase coexistence’ [8].

We note that the $s$-ensemble is time-translationally invariant (TTI) only for times $0 \ll t \ll t_{obs}$, with deviations from TTI behaviour [8] near the initial and final times. These boundary effects enhance the contribution of the active phase to $Z(s, t_{obs})$, so that for fixed $N$ we expect [22] that $s^* = s_N + O(1/t_{obs})$, consistent with Fig. 1(b). The scaling of $\chi^*$ 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 $s$ [19].

We characterise the dynamical behaviour of the ROM in the $s$-ensemble via the autocorrelation function, $C_s(t) = \langle N^{-1} \sum_i \sigma_i(t') \sigma_i(t) \rangle_s$, which is independent of $t'$ for $0 \ll t' < t + t' \ll t_{obs}$ [8]. Fig. 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 $\tau$. 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 $q_{EA} \equiv \lim_{t \to \infty} C_s(t)$, with the limit taken after the limits of large $N$ and $t_{obs}$. We now show that systems realising the 1-RSB scenario have a first-order dynamical transition from a ‘paramagnetic state’ with $q_{EA} = 0$ to a ‘spin glass’ with finite $q_{EA}$, as $s$ is increased through zero. This is consistent with Figs. 1a and 2, since the ROM realises this scenario.

Our discussion rests on the existence of a large number of metastable states, which can be studied within the TAP approach [12, 16, 17]. The presence of TAP states is sufficient to prove the existence of a space-time phase transition. Let $\mathcal{W}$ 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 $\mathcal{W}$: There is a spectrum of fast rates larger than some cutoff $\gamma_1$ and a spectrum of slow rates smaller.
than a second cutoff $\gamma_s < \gamma_t$. On starting in a given configuration, the system relaxes quickly into a metastable (TAP) state in a time of order $\gamma_t^{-1}$. However, transitions between these states occur much more slowly, taking a time of order $\gamma_s^{-1}$. Then, for $\gamma_t^{-1} \ll t_{\text{obs}} \ll \gamma_s^{-1}$, the time evolution operator of the system is a projection operator onto the TAP states:

$$e^{W_{\text{obs}}} = \sum_{\alpha} |P_\alpha\rangle\langle Q_\alpha| + O(e^{-\gamma_t t_{\text{obs}}}) + O(\gamma_s t_{\text{obs}}), \quad (3)$$

where $|P_\alpha\rangle$ describes the (metastable) equilibrium distribution within state $\alpha$, and $\langle Q_\alpha|$ gives the probabilities of relaxation into state $\alpha$ [20]. This result was used in [17], where the trace of $e^{W_{\text{obs}}}$ 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 $\mathcal{W}(s)$ [14, 21], such that $\mathcal{W}(0) = \mathcal{W}$. Further, the largest eigenvalue of $\mathcal{W}(s)$ can be estimated variationally [5], so that $\psi(s) \geq \langle \Psi | e^{s/\mathcal{T}} e^{\mathcal{W}(s)} | \Psi \rangle$ for any trial state $|\Psi\rangle$, with $\hat{E}$ being the energy operator of the system (we take $k_B = 1$). For small $s$, we use the variational basis $|P_\alpha\rangle$, arriving at

$$\psi(s) \geq \psi_{\text{var}}(s) = -N \min_{\alpha} [s k_\alpha] + O(\gamma_s) + O(s^2) \quad (4)$$

where $k_\alpha$ is the average value of the activity density $K/(Nt_{\text{obs}})$ for trajectories at (metastable) equilibrium in state $\alpha$. For $\gamma_s \ll |s| \ll \gamma_t$, the bound is saturated [22], and

$$k(s) \approx \theta(s) \min_{\alpha} [k_\alpha] + \theta(-s) \max_{\alpha} [k_\alpha], \quad (5)$$

where $\theta(s)$ is the step function. In the 1-RSB scenario, the slow rate $\gamma_s$ vanishes in the limit of large-$N$. Taking this limit, followed by a limit of large $t_{\text{obs}}$, Eq. (5) holds as $|s| \to 0$. Hence, if the states $\alpha$ cover a finite range of $k_\alpha$ then $k(s)$ is discontinuous at $s = 0$. Thus, if $\gamma_t$ is finite and $\gamma_s \to 0$, there is a first-order dynamical transition at $s = 0$, similar to that seen in KCMs [5]. The prediction of Eq. (5) and the numerical observations of Figs. 1 and 2 constitute the key results of this paper: for $T_d < T < T_o$, the ROM has a first-order space-time phase transition at $s = 0$.

In thermodynamics, first-order phase transitions are characterised by singular responses to boundary fields. We take $s = 0$ and $T_d < T < T_o$, 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 $q_{\text{EA}}$ [14]. 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 [3, 23].

So far we have considered only $T_d < T < T_o$. For temperatures above the onset temperature, $T > T_o$, metastable states are no longer infinitely long-lived and the slow rate $\gamma_s$ remains finite even as $N \to \infty$. It follows that $k(s)$ is continuous at $s = 0$. In the absence of a diverging slow time scale associated with the operator $\mathcal{W}$, one might expect $k(s)$ to be analytic for all $s$ [19]. However, for $T > T_o$, analytic arguments [22] and numerical results both indicate a first-order dynamic phase transition between active and inactive phases that occurs at finite $s^*$. Fig. 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 [11, 21].

For $T < T_d$, the behaviour is subtle and we postpone a detailed discussion to later work [22]. In this regime, 1-RSB systems have ‘threshold’ states which are associated with aging behaviour [23]. The relaxation time within the paramagnetic state diverges, and the ‘gap’ $(\gamma_t - \gamma_s)$ vanishes. We evaluate the bound in Eq. (4) while excluding the paramagnetic state from the minimisation. The
for the existence of a first-order space-time phase transition and the onset of metastability, peratures between the dynamical transition temperature $T_d$, summarised in the ($s$, $T$) plane, and not from paramagnetic 'threshold' states. The active state is constructed from active metastable states that line is a first-order transition between active and inactive dynamics. $T < T_o$ but it now results in the ROM for numerical simulations. During the early stages of this work, RLJ was funded through the U.S. Office of Naval Research through grant No. N00014-07-1-068.

We thank D. Chandler and F. van Vlijland for helpful discussions, and RLJ thanks D.R. Reichman for suggesting the suitability of the ROM for numerical simulations. Our main conclusion is that dynamical phase coexistence between active and inactive phases is not restricted to idealised KCMs [8] but also present in atomistic liquids [9], and, as we have shown here, in spin-glasses. The $s$-ensemble is the natural method for studying inactive and metastable states and their consequences in glassy systems in general.

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 $T_o$. For $T > T_o$ 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. 4.

resulting bounds may not be saturated so the proof of Eq. 5 fails. However, as long as the minimisation contains states with a finite range of $k_n$, Eq. 1 establishes the existence of a first-order space-time phase transition for $T < T_d$, similar to that for $T > T_d$. Fig. 3(b) shows numerical results consistent with such a transition. 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.

The dynamical phase structure of the ROM is summarised in the ($s$, $T$) phase diagram of Fig. 4. For temperatures between the dynamical transition temperature and the onset of metastability, $T_d < T < T_o$, metastable states lead to a first-order dynamical phase transition at $s = 0$ (Fig. 4). Thus, the equilibrium ensemble of trajectories is associated with coexistence between active (ergodic) and inactive phases. Above $T_o$, 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 non-ergodic phase in which the activity $k(s)$ is larger than its equilibrium value $k(0)$ but $q_{EA} > 0$. 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 focussed on the ROM in this article, but Eqs. 4 and 5 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 idealised KCMs [8]...
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