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Super-Potts glass: A disordered model for glass-forming liquids

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We introduce a disordered system, the super-Potts model, which is a more frustrated version of the Potts glass. Its elementary degrees of freedom are variables that can take M values and are coupled via pairwise interactions. Its exact solution on a completely connected lattice demonstrates that, for large enough M, it belongs to the class of mean-field systems solved by a one-step replica symmetry breaking ansatz. Numerical simulations by the parallel tempering technique show that in three dimensions it displays a phenomenological behavior similar to the one of glass-forming liquids. The super-Potts glass is therefore a disordered model allowing one to perform extensive and detailed studies of the random first-order transition in finite dimensions. We also discuss its behavior for small values of M, which is similar to the one of spin glasses in a field.

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Glass-forming liquids have a very peculiar and rich phenomenology [1]. Dynamical correlation functions are characterized by a two-step relaxation, indicating that a finite fraction of degrees of freedom, e.g., density fluctuations, takes an increasingly longer time τ to relax. This time scale actually grows very rapidly—more than 14 orders of magnitude in a rather restricted window of temperatures—and can be fitted by the Vogel-Fulcher-Tamman law, hence suggesting a possible divergence at finite temperature. The slowing down of the dynamics is accompanied by the growing of dynamical correlations, which can be measured by a four-point susceptibility. This function displays at time τ a peak that grows with decreasing temperature and is related to the number of molecules that have to move in a correlated way in order to make the liquid flow.

One of the most influential results obtained in the field of glass transitions was the discovery by Kirkpatrick, Thirumalai, and Wolynes [2] that some—apparently unrelated—fully connected mean-field (MF) disordered systems, such as the Potts glass, display a phenomenology very similar to the one described above. This set the stage for an approach to the glass transition problem that combined disordered systems, and mode-coupling and Adam-Gibbs theories, and culminated in the development of the random first-order transition (RFOT) theory [3]. Although structural liquids do not explicitly contain quenched disorder in the Hamiltonian, they are frustrated and characterized by a very complicated rugged energy landscape. This is the key element they have in common with several disordered systems and that is at the origin of the relationship cited above. MF disordered systems divide in two classes: Some have a phenomenology similar to glass-forming liquids, and others to spin glasses. The former are the ones for which, in replica language, the one-step replica symmetry breaking (1RSB) approximation is exact [4]. For these models the relaxation time is known to diverge at a finite temperature, called T_d [5]. This transition was shown to be identical to the one predicted by the mode-coupling theory of glass transitions [1,6]. Below T_d ergodicity is broken. The phase space is fractured into a number of states $\mathcal{N}$ that is exponential with the size N of the system: $\mathcal{N} \propto e^{N\Sigma}$ (Σ is called the complexity or configurational entropy). The system undergoes a thermodynamic phase transition in the manner of Kauzmann at a smaller temperature $T_K < T_d$, where the configurational entropy vanishes and hence the number of states that dominate the Boltzmann measure becomes subexponential [7]. The order parameter for this transition is the overlap q measuring the similarity between two different replicas of the system (characterized by the same realization of the disorder). Its distribution $P(q)$ shows a single peak at $q_{\rm RS}$ for $T > T_K$ and two distinct peaks q_0 and q_1 for $T < T_K$. The lowest value, q_0, corresponds to the two replicas being in configurations belonging to two different amorphous states, whereas the higher one, q_1, to configurations belonging to the same state. There is, however, another class of MF disordered systems, the spin glasses, characterized by a quite different behavior. They display a continuous transition and are solved by the full replica symmetry breaking (FRSB) ansatz [8]. Dynamical correlation functions do not show any two-step relaxation, the four-point susceptibility is not peaked, $P(q)$ has continuous support below the transition, and $T_K = T_d$.

In view of the aforementioned analogy between structural glasses and MF 1RSB disordered models and of its relevance in RFOT theory, the numerical results on finite-dimensional counterparts of MF 1RSB systems were deceiving. It was found that the usual fate of these systems, once studied on finite-dimensional lattices, is to display either a continuous spin-glass transition or no transition at all. For instance, the MF Potts glass [9], the model from which RFOT theory originated, is characterized by a glass transition for any $p > 4$, where p is the number of values that Potts variables can take, but in three dimensions (3D) it does not show any transition for $p = 10$ [10]. The problem of the disappearance of the 1RSB phenomenology in finite dimensions could be a signal of the fragility of the 1RSB theory out of MF, and poses the question of the validity of RFOT in $D = 3$, as discussed in a series of papers by Moore and collaborators [11]. In a recent work [12] it was pointed out that the MF disordered models studied so far are not frustrated enough and even simple local fluctuations are enough to change their physics (see also Ref. [13]). This is well illustrated by their change of behavior on Bethe lattices, which provide a better mean-field-like approximation than fully connected models since they have finite connectivity and, hence, allow one to take into account the kind of local fluctuations present in finite dimensions. One should not conclude, however, that there are no models or results connecting MF theory to the behavior of finite-dimensional glass-forming liquids. Indeed, there are. Lattice glass models display the correct phenomenological behavior and they belong to the 1RSB class when solved on a Bethe lattice [14,15]. A particular form of a disordered five-spin model appears to behave correctly, too [16]. Finally, hard spheres in the limit of infinite dimensions do display a 1RSB transition [17]. However, from the point of view of the quest for finding simple finite-dimensional models displaying a glass transition, all these systems suffer from one or more limitations: They are either too hard to simulate in finite dimensions or they display a crystal phase that preempts the existence of the glass transition and deep supercooling or they do not have pairwise interactions, which makes them difficult to be analyzed in finite dimension, in particular, by real space renormalization group methods.

The aim of this Rapid Communication is to introduce and study a model that short circuits these problems and therefore offers a way to test RFOT theory and to answer questions on glassy physics. We call it the *super-Potts model*. It is similar to the modifications of the Potts glass introduced and studied in Refs. [18,19], which display a continuous transition and not the discontinuous one that we are looking for. Its degrees of freedom are variables that take M values, as in the usual Potts model, and its Hamiltonian reads

$$H(\{\sigma\}) = \sum_{(i,j)} \epsilon_{ij}(\sigma_i,\sigma_j)$$

with

$$\epsilon_{ij}(\sigma_i,\sigma_j) = \begin{cases} E_0 & \text{if} \quad (\sigma_i,\sigma_j) = (\sigma_i^*,\sigma_j^*), \\ E_1 & \text{otherwise,} \end{cases} \qquad (1)$$

and (σ_i^*,σ_j^*) are randomly drawn among the $M \times M$ possible couples (σ_i,σ_j) [independently for any couple of neighbors (i,j)]. For simplicity we will take $E_0 = 0$. We believe that singling out one random couple of variables per link makes the model more frustrated than the usual Potts glass [9] and the random-permutation versions of Refs. [18,19]. This is manifest in dimension $D = 1$. For these models, after having chosen the value of the first Potts variable, one can easily find sequentially the configuration of the next variable that minimizes the energy, because for each value of one variable, there exists a value of the neighboring one that can minimize the energy of the link. For the super-Potts glass, instead, there is only one particular configuration of both variables that minimizes the energy of the link, and not all the links can be satisfied simultaneously, even in $D = 1$. The super-Potts glass can be easily generalized to more complicated choices of the link energy, e.g., $\epsilon_{ij}(\sigma_i,\sigma_j)$ randomly drawn from a Gaussian distribution. In this way, in the limit $M \to \infty$, one ends up with a random energy model on each link [20,21].

We first present the analytical solution of the fully connected MF super-Potts glass. The corresponding Hamiltonian is the one in Eq. (1) with the sum over all pairs of Potts variables and the energy that scales as $E_1 = \frac{e_1}{\sqrt{N}}$, with $e_1 = O(1)$ for finite M and N being the total number of Potts variables. We sketch briefly the main steps of the computation and the results (more details can be found in the Supplemental Material [22]).

The replica method allows one to compute the average free energy $f = \overline{f_\epsilon}$, where the bar indicates the average over the disorder, in terms of the partition function of n replicas:

$$e^{-\beta N n f} = \lim_{n\to 0} \overline{Z^n} = \lim_{n\to 0} \overline{\sum_{\{\sigma\}} \prod_{i,j} e^{-\beta \sum_{a=1}^{n} \epsilon_{ij}(\sigma_i^a \sigma_j^a)}}. \qquad (2)$$

Repeating standard procedures [7], i.e., computing the average over the disorder, expanding the exponential for large N, and introducing Gaussian integrals over an auxiliary matrix Q_{ab}, we obtain

$$\overline{Z^n} \propto \sum_{\{\sigma\}} \int \prod_{a<b} dQ_{ab} e^{-NA(\mathbf{Q},\{\sigma\})} \propto \int d\mathbf{Q} e^{-NS(\mathbf{Q})}, \qquad (3)$$

with

$$A(\mathbf{Q},\{\sigma\}) = C \sum_{a<b} Q_{ab}^2 - \frac{1}{N} \sum_{a<b} 2C \sum_{i=1}^{N} \delta_{\sigma_i^a \sigma_i^b} Q_{ab}, \qquad (4)$$

where we defined $C = (\frac{\beta e_1}{M})^2$. We have chosen $e_1 = M$ in order to reabsorb the scaling with M of the critical temperature. The integral over $\mathbf{Q}$ is performed by the saddle-point method. The saddle-point value of Q_{ab}, defined by the equation $\frac{dA(\mathbf{Q},\{\sigma\})}{d\mathbf{Q}} = 0$, corresponds to the average value of the overlap $\frac{1}{N}\sum_i \delta_{\sigma_i^a \sigma_i^b}$. By using the replica symmetric (RS) ansatz, we restrict the possible forms of Q_{ab} to $Q_{ab} = q_{\mathrm{RS}}$. Within this assumption the saddle-point equation simplifies to

$$q_{\mathrm{RS}} = \int \prod_{\tau=1}^{M} \frac{dh_\tau}{\sqrt{4\pi}} e^{-\frac{h_\tau^2}{4}} \frac{\sum_{\tau=1}^{M} e^{2\sqrt{Cq_{\mathrm{RS}}}h_\tau}}{\left(\sum_{\tau=1}^{M} e^{\sqrt{Cq_{\mathrm{RS}}}h_\tau}\right)^2}.$$

Here and in the following, we shall solve these kinds of M-dimensional integrals by the Monte Carlo method. Note that even when the RS solution is the correct, stable one, q_{RS} is different from zero. In order to analyze whether the RS solution is the correct one, we have also studied its local stability by diagonalizing the Hessian of the action: $G_{ab,cd} = \frac{d^2 S(Q_{ab})}{dQ_{ab} dQ_{cd}}|_{Q_{ab}=q_{\mathrm{RS}}}$ [23]. One eigenvalue is always larger than 0, while the other one becomes negative at $T_{\mathrm{RS}}(M)$, indicating that the RS solution becomes unstable at low temperature. The values of $T_{\mathrm{RS}}(M)$ are listed in Table I for $M = 4,10,20,50$. Below $T_{\mathrm{RS}}(M)$ one necessarily has to look for a RSB solution. The next step is therefore to assume a 1RSB ansatz [4] for the matrix Q_{ab}, which is parametrized by three parameters, q_0, q_1, $0 \leqslant m \leqslant 1$. We are interested in finding T_d,T_K and deciding whether the transition is continuous or discontinuous; all this information can be obtained in the limit $m \to 1$ [24]. In this

TABLE I. β_{RS}, β_d, β_k, and the difference $q_1 - q_0$ at the dynamical transition for different values of M for the fully connected MF version of the super-Potts model.

M	β_{RS}	β_d	β_k	$q_1(\beta_d) - q_0(\beta_d)$
4	2.0841(9)	2.07(3)	2.07(3)	0
10	1.9658(6)	1.949(12)	1.949(12)	0
20	2.306(1)	2.215(4)	2.229(1)	0.2623(1)
50	3.255(6)	2.589(7)	2.665(3)	0.5772(7)

case, $q_0 = q_{\rm RS}$ and the saddle-point equation on q_1 reads

$$q_1 = \int \prod_{\tau=1}^{M} \frac{d\eta_\tau}{\sqrt{4\pi}} \frac{e^{-\frac{\eta_\tau^2}{4}}}{\sum_{\tau=1}^{M} e^{C(q_1-q_{\rm RS})+\sqrt{Cq_{\rm RS}}\eta_\tau}} \times \int \prod_{\tau'=1}^{M} \frac{dh_{\tau'}}{\sqrt{4\pi}} e^{-\frac{h_{\tau'}^2}{4}} \frac{\sum_{\tau'=1}^{M} e^{2(\sqrt{C(q_1-q_{\rm RS})}h_{\tau'}+\sqrt{Cq_{\rm RS}}\eta_\tau)}}{\sum_{\tau'=1}^{M} e^{\sqrt{C(q_1-q_{\rm RS})}h_{\tau'}+\sqrt{Cq_{\rm RS}}\eta_\tau}}.$$

Note that $q_1 = q_{\rm RS}$ is always a solution. As usual, we locate T_d as the highest temperature at which one finds a solution $q_1 \neq q_0$ and T_K as the temperature at which the configurational entropy vanishes [25]. We found that for large values of M ($M = 20,50$), q_1 emerges discontinuously from q_0, and $T_K(M) < T_d(M)$, signaling that the transition is 1RSB, i.e., glass-transition-like. For smaller M ($M = 4,10$), instead, q_1 emerges continuously from q_0 and $T_K(M) = T_d(M)$, meaning that the transition becomes continuous and similar to the one of MF spin glasses in a field, i.e., of FRSB type. The difference between q_0 and q_1 at T_d grows for larger M, indicating that increasing M indeed favors structural glasslike behavior. The values of $T_d(M)$, $T_K(M)$, and $q_1 - q_0$ at T_d are listed in Table I. In agreement with previous results, for $M = 4$ and 10, the critical temperatures are compatible within the error with $T_{\rm RS}$ [26].

As discussed previously, three-dimensional glass models may behave quite differently from their MF counterparts. It is therefore crucial to check that the super-Potts glass still behaves as a glass beyond MF. To this aim, we performed Monte Carlo (MC) numerical simulations of the model on a cubic lattice. We use the parallel tempering algorithm [27] to thermalize the system at low temperatures, running it simultaneously at 30 different temperatures. Four replicas have been simulated in parallel, letting them evolve independently with the same realization of disorder. We measure the overlap q between two of them, replicas a,b, as $q_{ab} = \frac{1}{N}\sum_{i=1}^{N} \delta_{\sigma_i^a,\sigma_i^b}$. We check the equilibration by dividing the first measurements into bins with a logarithmically growing size, and we assume that the system has reached the equilibrium when the probability distribution of the overlap $P(q)$ between the first two replicas is equal to $P(q)$ of the second two replicas inside the last bin, and with respect to the precedent bin (practically, we check the first four moments of q). Equilibration time is of the order of 10^8 MC steps for systems with $M = 30$ and size $L = 8$. Once the system is thermalized, we run standard MC simulations to measure the dynamical correlation functions. Disorder averages were performed over 30 samples, while thermal ones over 100 trajectories. The behavior of the two times correlation (the angle brackets indicate the thermal average),

$$C(t) = \frac{1}{N}\overline{\sum_i \langle \sigma_i(0)\sigma_i(t)\rangle},$$

is shown in Fig. 1 for $M = 30$ [28]. By lowering the temperature, the two-step relaxation characteristic of glass-forming liquids emerges (for $M = 30$, the true plateau, corresponding to the peak of the susceptibility, is preceded by a first plateau that saturates at low enough temperature). Note that the asymptotic value of $C(t)$, $C(\infty) \equiv q_0$, is nonzero since the super-Potts glass, as many other disordered models introduced previously [9,18,19], has no symmetry precluding q_0 from being different from zero (in consequence, the two-step relaxation emerges on top of q_0) [29]. The value of q_0 grows, lowering the temperature, as found also in the MF model, starting from $q_0 = 1/M$ at $T = \infty$. For small values of M, instead, one finds a relaxation similar to the one of spin glasses in a field, as shown in the inset for $M = 4$. In Fig. 2 we show that the evolution of the four-point susceptibility $\chi_4(t)$, defined as

$$\frac{1}{N}\sum_{i,j}\overline{(\langle\sigma_i(0)\sigma_i(t)\sigma_j(0)\sigma_j(t)\rangle - \langle\sigma_i(0)\sigma_i(t)\rangle\langle\sigma_j(0)\sigma_j(t)\rangle)},$$

confirms this trend: $\chi_4(t)$ is peaked, its maximum takes place at the time at which the correlation escapes from the plateau, and grows when lowering the temperature, as it happens for supercooled liquids. This behavior, present for $M = 30$, is

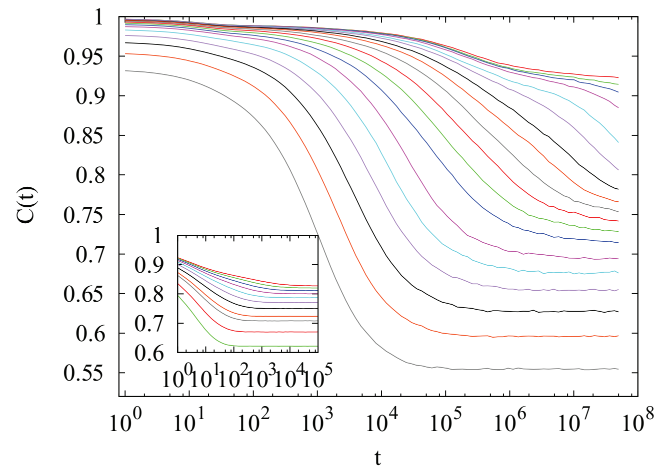

FIG. 1. (Color online) Two-time correlation function for systems with $M = 30$ and $L = 8$ (main panel, inverse temperature β equally spaced in [0.28,0.85], from left to right) and with $L = 12$ $M = 4$ (inset, β equally spaced in [0.76,1.09], from left to right). Note that the characteristic two-step relaxation emerges on top of the asymptotic value $C(\infty) = q_0 > 0$.

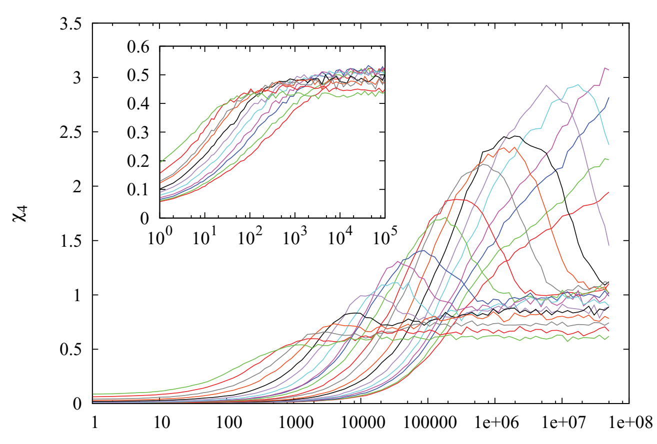

FIG. 2. (Color online) Four-point susceptibility for a system with $L = 8$, $M = 30$ (main panel) and with $L = 12$, $M = 4$ (inset). Temperatures as in Fig. 1.

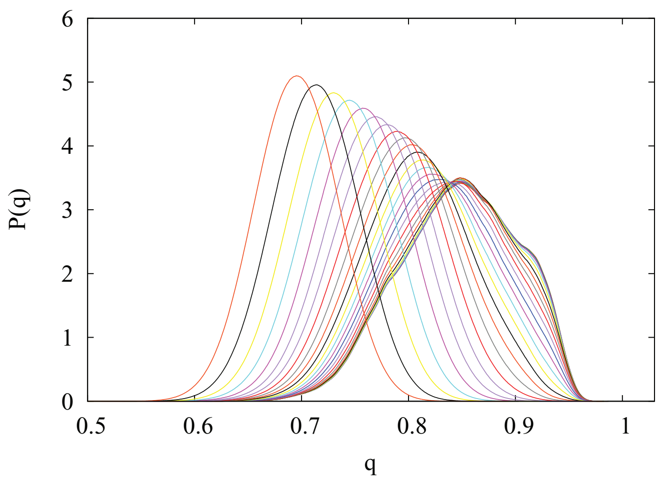

FIG. 3. (Color online) $P(q)$ for a system with $L = 10$, $M = 20$. β equally spaced in [0.55,1.3] (from left to right).

markedly different from the one shown in the inset for $M = 4$. For M's in between the two presented values the system actually seems to show a mixed behavior; for instance, $\chi_4(t)$ shows a peak but also a growing plateau. We also studied the overlap distribution $P(q)$. Although of course one would need much larger sizes to provide convincing evidence of a phase transition, our results, shown in Fig. 3, suggest that if there is a transition, then it should be discontinuous already for $M = 20$, since a second peak seems to appear discontinuously at small temperatures as if a 1RSB transition were indeed taking place. Overall, our numerical results indicate that at large M ($M \gtrsim 20$) the super-Potts glass behaves similarly to glass-forming liquids, whereas for smaller M's analogously to a spin glass in a field, in agreement with the MF treatment presented before.

In conclusion, we introduced a model, the super-Potts glass, and showed that is an example of a glassy disordered system with pairwise interactions, solved by a 1RSB ansatz at the MF level, and which has, in three dimensions, a phenomenological behavior strongly reminiscent of glass-forming liquids. In particular, it shows stretching (nonexponential behavior) and two-step relaxation for the correlation function, a time for the relaxation from the plateau that seems to diverge at finite temperature, a growing peak in the four-point correlation function, and a discontinuous peak appearing in the $P(q)$. The glassy behavior is only found for sufficiently high numbers M of values that the Potts variables can take. This is reasonable if we think of a real-world structural glass, where the degrees of freedom, i.e., the position of particles, can take infinite values. Compared to previous models for which the glassy behavior does not survive in finite dimensions, the super-Potts glass is more frustrated and this enhances its stability. Indeed, we computed the so-called surface energy cost Y to disrupt amorphous order, as was done in Ref. [12], and found a value of Y/T_K, which is an order of magnitude higher than in previous models for large values of M, e.g., $M = 50$. There are several extensions of our work worth pursuing further. First, it would be interesting to clarify how the transition between the glasslike to the spin-glass-like behavior induced by decreasing the value of M takes place, both in mean field and in finite dimensions. A possible scenario, inspired by the behavior of the $2+4$ spin MF model, is the following [30]: Whereas at small M there is a pure FRSB phase and at large M a pure 1RSB phase, at intermediate M, by decreasing the temperature, there is first a RS to FRSB transition, and then, lowering the temperature further, there is a transition to a $1+$FRSB in which $P(q)$ has a continuous part but also develops a discontinuous peak. This is consistent with the fact that for intermediate values of M the correlation function and the four-point susceptibility show mixed features that are characteristic of both the 1RSB and FRSB phases. Another research direction for future studies is solving exactly the super-Potts model on Bethe lattices. This would provide a good approximation to the 3D case since, as we found in numerical simulations, the behavior on cubic and Bethe lattices with connectivity $C = 6$ is qualitatively and also quantitatively similar. The exact solution of models on the Bethe lattices can be obtained via the cavity method, which in the case of the super-Potts glass, however, is particularly challenging [31]. It could be also interesting to apply the trick used in Ref. [18] to obtained a modified version of the model that could have a symmetric $P(q)$, allowing an easier thermalization and more extensive numerical simulations. Finally, another interesting route to follow in order to clarify the behavior of the 3D model is by performing a renormalization group analysis. Since the model has pairwise interactions, this can be naturally done by the Migdal-Kadanoff approximation.

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