Evidence of a glass transition in a 10-state nonmean-field Potts glass

Ruben S. Andrist, Derek Larson, and Helmut G. Katzgraber^{3, 1}

¹ Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland

² Department of Physics, National Taiwan University, Taipei, Taiwan

³ Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843-4242, USA

(Dated: June 14, 2018)

Potts glasses are prototype models that have been used to understand the structural glass transition. However, in finite space dimensions a glass transition remains to be detected in the 10-state Potts glass. Using a one-dimensional model with long-range power-law interactions we present evidence that a glass transition below the upper critical dimension can exist for short-range systems at low enough temperatures. Gaining insights into the structural glass transition for short-range systems using spin models is thus potentially possible, yet difficult.

PACS numbers: 75.50.Lk, 75.40.Mg, 05.50.+q

I. INTRODUCTION

Due to their fascinating properties such as aging, memory effects and ergodicity-breaking transitions, as well as industrial applications, structural glasses, supercooled liquids and polymers have received considerable attention recently. In particular, when the temperature is decreased, they undergo a dynamic transition [1–3] below which the particle-density correlation length does not decay to zero in the long-time limit and the evolution becomes nonergodic. However, this transition is not associated with any thermodynamic singularity. Hence the system "freezes" in a portion of phase space. There is a second transition at a lower temperature [4, 5] which can be associated with a thermodynamic singularity and which can be related to a possible ideal glass transition. Despite ongoing efforts, the structural glass transition remains to be fully understood.

The p-state Potts glass [6–11] is one of the most versatile models in statistical physics: For p = 2 states it reduces to the well-known Edwards-Anderson Ising spin glass [12], a workhorse in the study of disordered magnetic systems. For p=3 it can be used to model orientational glasses [13], while for p=4 the Potts glass can be used to model quadrupolar glasses. For large p > 4 and no disorder the model shows a first-order transition. In particular, infinite-range Potts glasses with p > 4 exhibit a transition from ergodic to nonergodic behavior [6–11], as well as an additional static transition at a lower temperature. In fact, the equations describing the system's dynamics near the transition are mathematically related [14–16] to the equations of mode-coupling theory, which describe the behavior found in structural glasses and supercooled liquids. Therefore, studying the Potts glass with large p could provide, in principle, some insights into the mechanisms governing the structural glass transition. However, this beneficial relationship seems to only work when the model is infinite ranged [17]. The existence of a transition in finite-dimensional systems remains to be proven [18, 19]. Not only are hypercubic lattices with large space dimension hard to study numerically, recent

work [20, 21] suggests that if there is a transition for large p it would occur at very low temperatures.

In this work we simulate the 10-states Potts glass on a one-dimensional ring topology with power-law interactions. This allows us to effectively tune the range of the interactions and therefore the (effective) space dimension for large linear system sizes. Our results suggest that 10-state Potts glasses should have a very low finite-temperature transition for finite space dimensions.

The paper is structured as follows. In Sec. II we introduce the model and observables. Furthermore, we outline the details of the numerical simulations. Section III summarizes our findings, followed by concluding remarks.

II. MODEL AND OBSERVABLES

We study a one-dimensional Potts glass with longrange power-law interactions [22, 23] and Hamiltonian $\mathcal{H} = -\sum_{i,j} J_{ij} \delta_{q_i,q_j}$, where $q_i \in \{1,\ldots,10\}$ are 10state Potts spins on a ring of length L to enforce periodic boundary conditions and $\delta_{x,y} = 1$ if x = y and zero otherwise. The sum is over all spins and the interactions J_{ij} are given by $J_{ij} = \varepsilon_{ij}/r_{ij}^{\sigma}$, where ε_{ij} are Normal distributed with mean J_0 and standard deviation unity. $r_{ij} = (L/\pi)\sin[(\pi|i-j|)/L]$ represents the geometric distance between the spins on the ring. For the simulations we express the Potts glass Hamiltonian using the simplex representation where the 10 states of the Potts spins are mapped to the corners of a hypertetrahedron in nine space dimensions. The state of each spin is therefore represented by a nine-dimensional unit vector \vec{S}_i taking one of the 10 possible values satisfying the condition $\vec{S}^{\mu} \cdot \vec{S}^{\nu} = [p/(p-1)](\delta_{\mu,\nu} - 1)$ with $\{\mu,\nu\}\in\{1,2,\ldots,10\}$. In this representation the Potts glass Hamiltonian is given by $\mathcal{H} = -\sum_{i,j} \tilde{J}_{ij} \vec{S}_i \cdot \vec{S}_j$ with $J_{ij} = J_{ij}(p-1)/p$. In the limit when $\sigma \to 0$, when the system is infinite ranged (Sherrington-Kirkpatrick limit), we obtain $T_c(\sigma=0)=1/(p-1)$.

The merit of the long-range one-dimensional model lies in emulating a short-range topology of varying dimensionality, depending on the power-law exponent: For $\sigma \leq 2/3$ the model is in the mean-field long-range 10-state Potts universality class and, in particular for $\sigma \leq 1/2$ in the infinite-range universality class. However, for $2/3 < \sigma < 1$ the model is in a nonmean-field universality class with a finite transition temperature T_c . It can be shown [22] that $\sigma = 2/3$ corresponds exactly to six space dimensions for a hypercubic lattice. Therefore, σ values between 1/2 and 2/3 allow us to effectively study [22, 23] a short-range hypercubic Potts glass above the upper critical dimension $d_u = 6$, whereas when $\sigma > 2/3$ we effectively study a model with a space dimension below six dimensions. Thus, by studying the one-dimensional model we can infer if a transition should be present for the corresponding short-range hypercubic Potts glass.

The presence of a transition is probed by studying the two-point finite-size correlation length [24]. We measure the wave-vector-dependent spin-glass susceptibility [25]

$$\chi_{\rm SG}(\mathbf{k}) = N \sum_{\mu,\nu} [\langle |q^{\mu\nu}(\mathbf{k})|^2 \rangle]_{\rm av}, \qquad (1)$$

where $\langle \cdots \rangle$ denotes a thermal average, $[\cdots]_{av}$ an average over the disorder and

$$q^{\mu\nu}(\mathbf{k}) = \frac{1}{N} \sum_{i} S_i^{\mu(\alpha)} S_i^{\nu(\beta)} e^{i\mathbf{k}\cdot\mathbf{R}_i}, \qquad (2)$$

is the spin-glass order parameter computed over two replicas (α) and (β) with the same disorder. The two-point finite-size correlation length is then given by

$$\xi_L = \frac{1}{2\sin(k_{\min}/2)} \left[\frac{\chi_{SG}(\mathbf{0})}{\chi_{SG}(\mathbf{k}_{\min})} - 1 \right]^{1/(2\sigma-1)},$$
 (3)

where $\mathbf{k}_{\min} = 2\pi/L$ is the smallest nonzero wave vector. According to finite-size scaling [25]

$$\xi_L/L^{\nu/3} = \mathcal{X}[L^{1/3}(T - T_c)] \quad (1/2 < \sigma \le 2/3), \quad (4a)$$

$$\xi_L/L = \mathcal{X}[L^{1/\nu}(T - T_c)] \quad (2/3 < \sigma),$$
 (4b)

where ν is the critical exponent for the correlation length and T_c the critical temperature. For $\sigma < 2/3$, $\nu = 1/(2\sigma - 1)$.

In practice, there are corrections to scaling to Eqs. (4) and so data for different system sizes do not cross exactly at one point as implied by the finite-size scaling expressions. The crossings between pairs of system sizes L and 2L shift with temperature and tend to a constant for $L \to \infty$. In general, $T_c^* = T_c^\infty + b/L^\theta$ with $\theta = 1/\nu + \omega$. Here we find empirically that $1/\nu + \omega \approx 1$. We fit $T_c^*(L, 2L)$ with high probability to a linear function in 1/L. The intercept with the vertical axis after the fit determines a lower bound for the transition temperature. Error bars are determined via a bootstrap analysis.

To obtain a better understanding of the corrections to scaling we also measure the spin-glass susceptibility

TABLE I: Parameters of the simulations for different exponents σ . $N_{\rm sa}$ is the number of samples, $N_{\rm sw}$ is the total number of Monte Carlo sweeps, $T_{\rm min}$ is the lowest temperature simulated, and N_T is the number of temperatures used in the parallel tempering method for each system size L.

σ	L	$N_{ m sa}$	$N_{ m sw}$	T_{\min}	N_T
0.60	32, 48, 64, 96	4000	2^{20}	0.054	41
0.60	128, 192	2400	2^{21}	0.054	41
0.60	256	500	2^{22}	0.054	41
0.60	512	200	2^{22}	0.054	41
0.75	32, 48, 64, 96	4000	2^{20}	0.030	41
0.75	128	1600	2^{22}	0.030	41
0.75	192	1600	2^{24}	0.030	41
0.75	256	500	2^{26}	0.030	41
0.85	32, 48, 64, 96	4000	2^{20}	0.018	61
0.85	128	1600	2^{22}	0.018	61
0.85	192	1600	2^{24}	0.025	41
0.85	256	500	2^{26}	0.025	41
0.65	200	500		0.025	4.

[Eq. (1) with $\mathbf{k} = 0$]. The finite-size scaling of the spinglass susceptibility $\chi_{\rm SG}$ is given by

$$\chi_{\rm SG}/L^{1/3} = \mathcal{C}[L^{1/3}(T - T_c)] \quad (1/2 < \sigma \le 2/3), \quad (5a)$$

$$\chi_{\rm SG}/L^{2-\eta} = \mathcal{C}[L^{1/\nu}(T - T_c)] \quad (2/3 < \sigma) \,.$$
 (5b)

In general, the exponent η has to be known a priori to precisely determine the location of T_c . However, for the one-dimensional model $2 - \eta = 2\sigma - 1$ for $\sigma > 2/3$ exactly and so $\chi_{\rm SG}/L^{2-\eta}$ can be treated as a dimensionless quantity similar to the two-point correlation length.

To prevent ferromagnetic order [6, 7] we set the mean of the random interactions to $J_0 = -1$ [18] in our simulations. This suppresses the ferromagnetic susceptibility $\chi_m = N \sum_{\mu} [\langle |m^{\mu}|^2 \rangle]_{\rm av} \ [m^{\mu} = (1/N) \sum_i S_i^{\mu}]$. We discuss the case where $J_0 = -1$ in more detail below.

The simulations are done using the parallel tempering Monte Carlo technique [26]; simulation parameters are shown in Table I. Equilibration is tested by using an exact relationship between the energy and four-spin correlators (link overlap) [27] when the bond disorder is Gaussian, suitably generalized to Potts spins [19] on a one-dimensional topology [28].

III. RESULTS

Our results are summarized in Fig. 1. The main panels in the left column show data for the finite-size correlation length as a function of temperature for (a) $\sigma=0.60$, (c) 0.75, and (e) 0.85. The insets show the corresponding data for the scaled dimensionless susceptibility. In all cases data for different system sizes cross, indicating the presence of a transition. To better quantify the thermodynamic behavior, we show in the right column the scaling of the crossing between successive system size pairs $T^*(L,2L)$ as a function of 1/L. The data can be well fit by a linear function; the intercept with the vertical axis corresponding to the thermodynamic limit. For all σ studied we find finite values for the thermodynamic glass

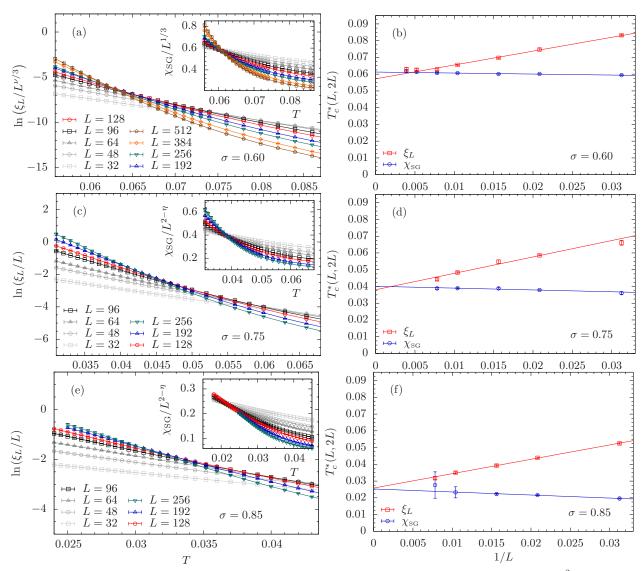


FIG. 1: (Color online) Panels (a), (c) and (e) show the correlation length ξ_L/L (inset: susceptibility $\chi_{\rm SG}/L^{2-\eta}$) as a function of temperature T for different system sizes L. Panel (a) shows data for $\sigma=0.60$ (mean-field regime) where a transition is expected [29] [note that here $\nu=1/(2\sigma-1)$]. Panels (c) and (e) show data for $\sigma=0.75$ and $\sigma=0.85$, respectively, which correspond to a space dimension below the upper critical dimension. A transition for low yet finite temperature is clearly visible. Panels (b), (d) and (f) show the crossing temperatures $T_c^*(L, 2L)$ of successive pairs of system sizes for different exponents σ [(b) 0.60; (d) 0.75; (f) 0.85]. The crossings for both ξ_L/L and $\chi_{\rm SG}/L^{2-\eta}$ are well approximated by a linear behavior in 1/L. Despite small deviations between the estimates for both quantities, for all σ values studied $T_c(\sigma) > 0$. In particular, we estimate $T_c(0.60) = 0.060(4)$, $T_c(0.75) = 0.040(3)$ and $T_c(0.85) = 0.025(3)$. Note that the data for $\sigma=0.60$ show a deviation from the linear behavior for the largest system sizes studies. However, both data sets agree and therefore suggest that the thermodynamic limit might have been reached.

transition. These findings for the long-range model with power-law interactions imply that the 10-state mean-field Potts glass, for $d_{\rm u} < d < \infty$ space dimensions, has a stable glass phase at finite temperatures. In addition, our data for $\sigma > 2/3$ indicate that short-range Potts glasses with a space dimension below the upper critical dimension should also have a finite transition temperature, albeit at very low T [30].

Recently, Alvarez Baños et al. [21] performed a thorough study of a three-dimensional Potts glass with $p \leq 6$, bimodal disorder and $J_0 = 0$. Their main result is that T_c

decreases with an increasing number of states p and suggests that for 10 states T_c should be strongly suppressed, in agreement with our results. In addition, Alvarez Baños et al. [21] claim that (1) only weak ferromagnetic order is visible when $J_0 = 0$, (2) that the complexity of the simulations is much higher when $J_0 = 0$, (3) that setting $J_0 = -1$ could impact the presence of the glass transition, and (4) that the transition could be first order.

We have examined these claims using the one-dimensional model with Gaussian disorder and find that (1) ferromagnetic order grows considerably when $J_0 = 0$

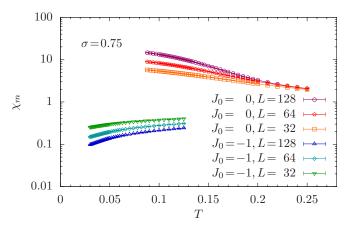


FIG. 2: (Color online) Ferromagnetic susceptibility χ_m as a function of temperature T for different system sizes. Ferromagnetic order is strongly suppressed for $J_0 = -1$ in comparison to the $J_0 = 0$ case.

at low enough temperatures (see Fig. 2) and (2) the complexity of the simulations is not affected by shifting the mean of the interactions. With respect to point (3), we do find, however, that the transition temperatures are reduced by approximately a factor of 2-3 when $J_0 = -1$ in comparison to the simulations where $J_0 = 0$. Shifting the mean of the interactions therefore only quantitatively impacts the transition temperature. Finally, (4),

for the system sizes studied, the distribution functions of the energy show no double-peak structure that would be indicative of a first-order transition.

IV. CONCLUSIONS

Using a one-dimensional 10-state Potts glass with power law interactions, we present evidence suggesting that short-range finite-dimensional 10-state Potts glasses should exhibit a finite-temperature transition for low enough temperatures and large enough system sizes. Although corrections to scaling are large, we estimate that for all σ values studied $T_c(\sigma) > 0$. In particular, we conservatively estimate $T_c(0.60) = 0.060(4)$, $T_c(0.75) = 0.040(3)$, and $T_c(0.85) = 0.025(3)$. Larger system sizes might show a different behavior, however, the presented state-of-the-art simulations show strong evidence that short-range 10-state Potts glasses in high enough space dimensions should order.

Acknowledgments

We thank A. P. Young for numerous discussions. H.G.K. acknowledges support from the SNF (Grant No. PP002-114713). The authors acknowledge ETH Zurich for CPU time on the Brutus cluster.

- W. Götze and L. Sjögren, Rep. Prog. Phys. 55, 241 (1992).
- [2] C. A. Angell, Science **267**, 1924 (1995).
- [3] K. Binder, J. Baschnagel, W. Kob, and W. Paul, (cond-mat/0202337) (2002).
- [4] W. Kauzmann, Chem. Rev. 43, 219 (1948).
- [5] J. H. Gibbs and E. A. Di Marzio, J. Chem. Phys. 28, 373 (1957).
- [6] D. Elderfield and D. Sherrington, J. Phys. C 16, L497 (1983).
- [7] D. J. Gross, I. Kanter, and H. Sompolinsky, Phys. Rev. Lett. 55, 304 (1985).
- [8] H.-O. Carmesin and K. Binder, J. Phys. A 21, 4053 (1988).
- [9] M. Scheucher, J. D. Reger, K. Binder, and A. P. Young, Phys. Rev. B 42, 6881 (1990).
- [10] G. Schreider and J. D. Reger, J. Phys. A 28, 317 (1995).
- [11] O. Dillmann, W. Janke, and K. Binder, J. Stat. Phys. 92, 57 (1998).
- [12] S. F. Edwards and P. W. Anderson, J. Phys. F: Met. Phys. 5, 965 (1975).
- [13] K. Binder and J. D. Reger, Adv. Phys. 41, 547 (1992).
- [14] T. R. Kirkpatrick and P. G. Wolynes, Phys. Rev. A 35, 3072 (1987).
- [15] T. R. Kirkpatrick and D. Thirumalai, Phys. Rev. B 37, 5342 (1988).
- [16] T. R. Kirkpatrick and D. Thirumalai, J. Phys. A 22, L149 (1989).
- [17] W. Kob, C. Brangian, T. Stuhn, and R. Yamamoto, (cond-mat/0003282) (2000).

- [18] C. Brangian, W. Kob, and K. Binder, J. Phys. A 36, 10847 (2003).
- [19] L. W. Lee, H. G. Katzgraber, and A. P. Young, Phys. Rev. B 74, 104416 (2006).
- [20] A. Cruz et al., Phys. Rev. B 79, 184408 (2009).
- 21] R. Alaverz Baños et al., J. Stat. Mech. P05002 (2010).
- [22] G. Kotliar, P. W. Anderson, and D. L. Stein, Phys. Rev. B 27, 602 (1983).
- [23] H. G. Katzgraber and A. P. Young, Phys. Rev. B 67, 134410 (2003).
- [24] M. Palassini and S. Caracciolo, Phys. Rev. Lett. 82, 5128 (1999).
- [25] H. G. Katzgraber, D. Larson, and A. P. Young, Phys. Rev. Lett. 102, 177205 (2009).
- [26] K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. 65, 1604 (1996).
- [27] H. G. Katzgraber, M. Palassini, and A. P. Young, Phys. Rev. B 63, 184422 (2001).
- [28] H. G. Katzgraber and A. P. Young, Phys. Rev. B 72, 184416 (2005).
- [29] C. Brangian, W. Kob, and K. Binder, J. Phys. A 35, 191 (2002).
- [30] We have also studied the random-permutation Potts glass [31] (data not shown). However, equilibration turned out to be considerably harder and a reliable determination of the thermodynamic glass transition turned out to be impossible.
- [31] E. Marinari, S. Mossa, and G. Parisi, Phys. Rev. B 59, 8401 (1999).