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LETTER TO THE EDITOR

A simple model of a glass with finite-range periodic interactions

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Abstract. In this Letter we introduce a chopped Josephson junction array as a tractable short-ranged frustrated model of a glass without quenched disorder. We study its configurational entropy and conclude that there is no true thermodynamic phase transition at finite temperature.

1. Introduction

Recent studies of spin glasses and idealized periodic glasses with infinite-ranged interactions have led to a qualitatively clear picture of the existence and role of both thermodynamic and dynamical phase transitions and of the relevance of extensive configurational entropy of the glassy states [1–3]. The situation in (more conventional) systems with short-range interactions is less clear, with regard both to the quantitative formulation of the key questions and to their resolution. The purpose of the present Letter is to suggest and study a model short-ranged system without imposed quenched disorder which is simple enough to permit the definition and examination of concepts analagous to those of the infinite-ranged model studies, together with consideration of their implications.

A key concept is that glassy states have extensive configurational entropy and small attractor basins, while crystalline states are normally unique (or few) with large basins. In infinite-ranged systems these states are separated by barriers which grow with the system size, becoming impenetrable in the thermodynamic limit, making their analysis easier. The entropically relevant glassy states are bounded below in energy and a thermodynamic transition is consequently predicted at a temperature $T^* = (\mathrm{d}S_{\mathrm{conf}}(E)/\mathrm{d}E)^{-1}|_{E_c}$ where $S_{\mathrm{conf}}(E)$ is the configurational entropy at energy E and E_c is its energetic lower bound†. T^* is often identified as the analogue of the Kauzmann temperature which was originally introduced empirically [4] as the temperature at which the excess entropy of a super-cooled liquid would extrapolate to zero.

In infinite-ranged systems one can also demonstrate the existence of a well defined dynamical temperature, T_D, at which the system freezes into a glass. In conventional spin-glass models as typified by the Sherrington–Kirkpatrick model [5] these two temperatures are identical, but more generally $T_D \geqslant T^*$ [6] and indeed it is believed that $T_D > T^*$ is characteristic for infinite-ranged glasses without quenched disorder [7]. In real practical

† Strictly E should be replaced by the free energy restricted to motion within the state evaluated at T^*.

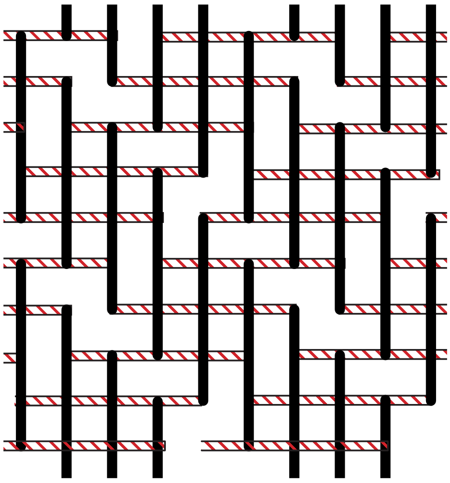

Figure 1. Sketch of the array. Each continuous horizontal or vertical section consists of a single superconducting wire with a constant superconducting phase angle along its length; to emphasize their difference, the horizontal wires are shown hatched while the vertical ones are solid. Weak Josephson junctions occur between horizontal and vertical wires where they cross.

(short-ranged) glasses experiments observe dynamical freezing over finite time-scales but the existence of a true dynamical transition is clouded by the impracticality of slow enough examination (see, for example, [8, 9]). It is even less clear whether a thermodynamic transition could take place at lower temperature in these systems. The situation is also difficult simulationally for typical atomic models because it is hard to distinguish adequately between different metastable states. The proposed model permits such distinctions and the study of the thermodynamic situation, albeit restricted to two dimensions, which might be expected [10] to be below the relevant critical dimension. This we report below; we do not address the dynamical transition of the model in this Letter.

2. Model

Our model is a periodic chopped Josephson junction array, based on the two-dimensional infinite-ranged periodic model introduced by us earlier [11] but with the wires cut with a period longer than the grid size and at 45° to the junction mesh (so as to maintain connectivity and frustration), as shown in figure 1. More specifically, the model consists of long wires in horizontal and vertical directions with Josephson contacts at the intersections and placed in a magnetic field. The cuts result in each section of wire having exactly m contacts with other sections in the orthogonal direction. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{ij} A_{ij} \exp\{2\pi \mathrm{i}\alpha x_i y_j / m\} z_i^* z_j + \mathrm{c.c.} \tag{1}$$

where $\alpha = m\ell^2 H/\Phi_0$, H is the field, ℓ is the spatial separation of neighbouring Josephson junctions and Φ_0 is the flux quantum $hc/2e$. Subscripts i and j label vertical and horizontal sections of wire with distances x_i, y_j from the corresponding boundary reference wires in units of the wire separation, $z_i = \mathrm{e}^{\mathrm{i}\phi_i}$ with $\{\phi_i\}$ the superconducting phase angles, and $A_{ij} = \{0, 1\}$ is the connectivity matrix, which is periodic in horizontal and vertical directions with period equal to the coordination number m of each section. The variables in the model are the ϕ_i, or equivalently the z_i. The Hamiltonian is symmetric under translations by m if and only if the flux through an elementary cell is integral; i.e. if $H(m\ell)^2 = n\Phi_0$; in this case we expect that the ground state is crystalline with an elementary cell of $2m$ wire sections. Our interest is particularly in cases where this condition is not true and glassy states are anticipated.

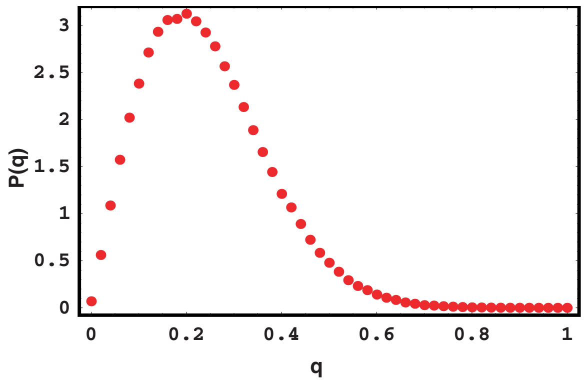

Figure 2. Distribution of overlaps (for $\alpha = 0.95$).

3. Method of solution

We have examined numerically several measures of the metastable states of the model (1) at zero temperature. In particular, we have studied the densities of states (and hence configurational entropies), basins of attraction and the inter-state overlap distribution as functions of α.

In order to find the metastable states and their basins we have used steepest descent searches in z-space starting from a wide range of random states (typically 10^4–10^6 starts were used), checking carefully in each case whether the resultant state is equivalent to or different from ones already obtained. For large m one expects a cross-over towards the fully connected problem [11], while for very small m the frustration is too small to get sufficiently many glassy states for good statistics in samples of size feasible for numerical analysis. We have concentrated on $m = 5$ to 7 as a reasonable compromise, here we show only results for $m = 5$, for which we collected the largest statistics for the largest system sizes. The results for $m = 7$ are quite similar for comparable system sizes. We have considered systems with N, the number of horizontal or vertical wires in a square array before cutting, in the range 5 to 30 which gives the total number of independent superconducting phase angles, N_s in the range 10 to 180.

4. Results

Initially it is necessary to check that we can differentiate unambiguously between states. To this end we have examined the distribution of overlaps $q^{ab} = (N_s)^{-1}|\Sigma_k z_k^{a*} z_k^b|$ between pairs of metastable states a, b (here $k = i$ or j); here the normalization $N_s = 2N^2/m$ is the number of wire sections. This is illustrated for $\alpha = 0.95$ in figure 2. We observe that the probability of finding two states with large overlap is very small; note that the maximum overlap possible is unity. Similar results are also found for other values of $\alpha \sim 1$. We are therefore able to take as a working rule to separate equivalent and different states whether their overlap is greater or less than some q_c (taken as ~ 0.9).

In figure 3 we display the normalized configurational entropy

$$S_{\text{conf}}(E) = \frac{1}{N_s} \ln \mathcal{N}(E) \tag{2}$$

where $\mathcal{N}(E)$ is the density of states at energy E, found in simulations for various system sizes. A study of a larger number of system sizes shows that the curves shift slightly with N but in an oscillatory manner and of reducing extent as N is increased, leading to the belief that the shapes shown are qualitatively representative of the thermodynamics limits and the shifts are boundary condition effects.

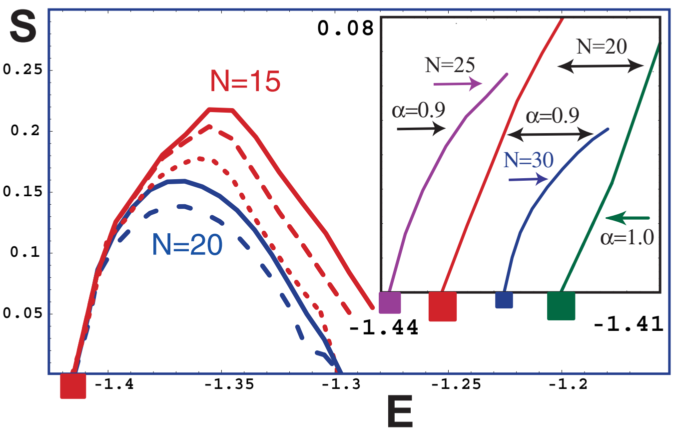

Figure 3. Configurational entropy, $S_{\mathrm{conf}}(E)$, per wire as found in simulations for $m = 5$ and different sizes, N, and for different numbers of random initial configurations, A. The curves shown in the main panel correspond to $\alpha = 0.95$. Notations are as follows (top to bottom): $N = 15$, $A = 10^6$ (solid), $A = 2 \times 10^5$ (dashed), $A = 5 \times 10^4$ (dotted) and $N = 20$, $A = 2 \times 10^5$ (solid), $A = 5 \times 10^4$ (dashed). Note the following features. The low-energy slope does not change with the increase in the number of attempts at fixed N, although the total number of states increases with A; this allows us to use a smaller number of attempts (crucial for large sizes) to calculate the leading edge of S_{conf}; the bin-sizes (same for $N = 15, 20$) are shown beneath. The insert shows a blow-up of the leading edge of S_{conf} with the bin-sizes indicated beneath. For a given size the steepness of the lower-energy slope is limited by the energy resolution, which in its turn is limited by the need for a finite number of states at a given size. An increase of the resolution becomes possible for larger sizes and the resulting slope increases with N. Here we show also data for $N = 25$ and $N = 30$ that were obtained for $A = 5 \times 10^5$ and $A = 2 \times 10^5$ initial configurations, respectively. We have verified that the data for $N = 25$ and $A = 2 \times 10^5$ and $A = 5 \times 10^5$ give indistinguishable leading-edge slopes, similar to the data for $N = 20$ shown in the main panel.

First, we confirm that the configurational entropy is indeed extensive. As with simulations of configurational entropy in other studies [15], it is difficult to ensure that all states have been found in the regions of high entropy and large E, especially as N is increased, leading to an underestimate for larger N in this region. However, consistency is obtained near the leading (lower E) edge. As is clear from figure 3, the shape of the lower-energy edge approaches its limiting value even for a moderate number of attempts. The reason for this is that lower-energy states have typically much larger attraction basins than the high-energy ones and thus can be found after only a moderate number of attempts. This observation allowed us to calculate the leading edge of S_{conf} for sizes up to $N = 30$ (which nevertheless required about 1000 hours of CPU time on a DEC Alpha workstation). The blow-up of the leading-edge behaviour is shown in the insert.

Second, we note (see the insert in figure 3) that change in α for a given N leads only to a curve displacement and does not result in any qualitative change. Increase of N has a much more dramatic effect on the exhibited slope of the leading edge (insert) which evidently grows with N. Technically, this is due to the fact that larger values of N allow us to decrease the bin-size (shown as boxes under the insert) without getting too much statistical noise. In other words, the need for finite bin-sizes for reasonable statistical weights leads to a finite resolution in energy and we believe that the observed finite slope at the leading edge of $S_{\mathrm{conf}}(E)$ is limited solely by this effect.

So, we conclude that in this model $S_{\mathrm{conf}}(E)$ has a very steep lower-energy edge, in striking contrast with the corresponding results for known infinite-range models (for example, for the

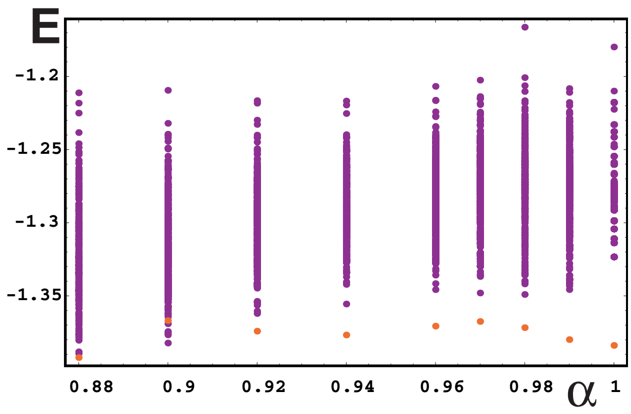

Figure 4. α-dependence of the energy bands for $N = 10$, $m = 5$.

infinite-connectivity version of the present model, see figure 3 of [3]). Our results suggest that in the large-N limit and for continuous E, the slope of $S_{\mathrm{conf}}(E)$ at its lower band edge is infinite. This implies the absence of a thermodynamic transition in this model.

We now remark on the α-dependence of our results. At small $\alpha \ll 1$ the frustration becomes less and the configurational entropy is decreased. This does not change the qualitative conclusions but makes it more difficult to obtain good state statistics on systems of reasonable size. As discussed above, for commensurate values of α the ground state is crystalline. However, there still remains a band of glassy states whose properties are expected to be similar to those for non-commensurate α. This expectation is borne out by the configurational entropy, as also illustrated in the insert to figure 3.

Another interesting observation concerns the relationship between the crystalline and glassy states. In figure 4 we show the evolution of the energy bands with α. We note that for α close to the special commensurate values the crystalline state continues and is well separated from the glassy band but as α deviates further it runs into the band. Since the basin of attraction of the crystalline state is large but that of any individual glassy state is small, the problem of finding a crystalline ground state is analogous to a *P* problem and that of finding a glassy ground state is analogous to *NP* (see, for example, [12]), while the transition between the two types of ground state with α is analogous to a *P* to *NP* transition (see, for example, [13, 14]).

Finally, we remark that the model studied here allows various modifications and variations; for instance, both vertical and horizontal wires can be cut along the lines in the same (1, 1) direction but shifted by a half period $(m/2)$ with respect to each other so to preserve the overall connectivity of the system. Studies of this case indicate that the main conclusion of this Letter, the infinite slope of the configurational entropy at low energy, is preserved in this system as well.

5. Conclusions

We have proposed a simple short-ranged frustrated model without quenched disorder and studied its glass and crystalline states. We have demonstrated that the configurational entropy of the glassy states is extensive and from its energy dependence have concluded that there is no true thermodynamic glass transition in this system. We have also shown the existence of a transition from crystalline to glassy ground state as a function of the frustration and have drawn analogies with *P*/*NP* transitions.

The system we have studied is two-dimensional so our result is inconclusive as to whether a thermodynamic glass transition is prevented by the finite range of interactions or by being below a lower critical dimension. The model could be extended to higher dimensions, either symmetrically or otherwise, although numerical study of large enough N would be harder and practical implementation would need further thought in the symmetric case.

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