Topological jamming of extended structures and the glass transition

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We propose a new scenario for glassy dynamics in frustrated systems with no quenched-in randomness, based on jamming of extended dynamical structures near a critical point. This route to a glassy state is demonstrated in a lattice model of fluctuating lines. Numerical simulations of the model show non-exponential relaxations and diverging energy barriers in the vicinity of a thermodynamic phase transition. A master equation for the coarse grained dynamics is constructed. It shows how topological jamming leads to the observed glassy dynamics.

Foams, granular materials and supercooled liquids, exhibit a transition from a flowing liquid phase to a jammed phase \[ \textcircled{1} \]. The dynamics of the flowing state near the transition are characterized by slow relaxations mediated by large-scale spatial rearrangements. These dynamical heterogeneities were dramatically demonstrated in recent experiments on colloids near the glass transition \[ \textcircled{2} \]. An important question posed by these observations is: What is the relation between length and time scales in a glass forming material?

The mode-coupling theory predicts a divergence of relaxation time scales with no dramatic growth of length scales. This is born out by experiments. A scaling theory of the glass transition, based on the existence of a zero-temperature critical point \[ \textcircled{3} \], leads to a similar conclusion about the relation between length and time scales. The frustration-limited domain theory \[ \textcircled{4} \] relates the origin of the dynamical heterogeneities and the activated nature of the dynamics to a critical point “avoided” due to frustrations imposed by competing interactions. Similarly, the random first-order transition theory \[ \textcircled{5} \] relies on the presence of frustration in glass formers and suggest that an unusual critical point is responsible for the dynamical behavior observed near the glass transition.

A phenomenological jamming phase diagram was recently proposed as a means of putting under one umbrella the whole spectrum of systems exhibiting dynamical arrest \[ \textcircled{6} \]. How, and if the above mentioned theories relate to jamming ideas remains to be explored. Here we propose a scenario for glassiness based on the interplay of jamming ideas and the same color has zero entropy density. By introducing an energy parameter that favors colorings in the zero entropy sector a phase transition can be induced in the model.

The frustration of the coloring model gives rise to naturally occurring extended structures in the system. Consider all the $A$ and $B$ colored bonds: there is one of each at every vertex, and therefore they must form loops. All the properties of the model, including the correlations of the microscopic variables, the colors, can therefore be traced back to the behavior of the ensemble of loops. These loops do not intersect, they have orientation ($ABAB \ldots$ versus $BABA \ldots$), and therefore they can be thought of as contour lines of a height field, that lives on the dual lattice \[ \textcircled{7} \] and provides an appropriate order parameter for the loop model.

The lattice with periodic boundary conditions, has a linear dimension $L$ with $2L^2$ sites and $3L^2$ bonds and the three lattice directions are indexed by $\alpha = 1, 2, 3$. We introduce a long-range interaction energy between $C$ colored bonds, with a parameter $\mu$ measuring the strength of this interaction:

$$ E = -\frac{\mu}{L^2} \sum_{\alpha=1,2,3} (2N_C^\alpha - L^2)^2. \quad (1) $$

Here $N_C^\alpha$ is the total number of $C$ bonds in the $\alpha$ direction. In the ground state all of the $C$ colored bonds are aligned in one of the three directions. This ordering effect acts against the entropic influence which tries to keep the number of colors homogeneous in all directions, and hence disordered. As the value of the coupling constant $\mu$ is increased from 0, the system undergoes a phase transition from a disordered to an ordered phase.

The phase transition is best described in terms of the height representation. In the disordered state, where the colors are randomly arranged, the corresponding surface is rough and untilted; Fig. \[ \textcircled{8} (a) \] shows the height of a typical coloring state. In the ordered state, with no extensive entropy, the surface is smooth and maximally tilted as shown in Fig. \[ \textcircled{8} (b) \].
A tilting transition of the surface occurs at $\mu = \mu_\ast$. The existence of a transition at a finite value, $\mu_\ast$ can be argued as follows. The entropy is maximum for a rough, untilted surface $\mathbf{F}$. Similarly from Eq. $[1]$ it follows that the energy is also maximized at zero tilt. Therefore the free energy, $F = E - S$, which is concave at $\mu = 0$, must change its curvature at a finite $\mu_\ast$. We numerically measured the equilibrium probability distribution of tilts for different values of $\mu$, and observed that the distribution becomes broader with increasing $\mu$. Quadratic fits indicate a $\mu_\ast \simeq 0.35 \pm 0.05$, at which the second derivative of the free energy function at zero-tilt vanishes. A tilting transition at a finite $\mu_\ast$ has been explicitly demonstrated in the two-color version of the current model $[8]$ lending further support to our argument.

In a unit microstep in our simulation, we randomly choose a site and choose either an $A-B$, $B-C$ or a $C-A$ loop passing through it, and we switch the colors on every alternate bond, using ordinary metropolis rules. For example, a $...ACAC...$ loop becomes a $...CACA...$ loop, with probability 1 if the energy change is non-positive and with rate $\exp(-\Delta E)$ when $\Delta E$ is positive. Since the energy function defined in Eq. $[1]$ depends on global numbers and not on local ones, it is easy to see that all local loop updates keep $\Delta E = 0$. Only when system spanning loops with nonzero winding numbers are chosen for update, does the possibility of $\Delta E \neq 0$ arise. Therefore, the tilting of the surface and hence the lowering of energy can only be brought about by updates of system-spanning loops. This path downhill in energy is blocked by barriers which lead to spectacularly slow dynamics near $\mu_\ast$, as will be shown below.

c. Simulation results: We measure the equilibrium, macroscopic tilt-tilt autocorrelation function, corresponding to the slowest mode in the system:

$$C(t) = \frac{\langle (\rho(t + t_o) - \langle \rho \rangle)(\rho(t_o) - \langle \rho \rangle) \rangle}{\langle (\rho(t_o) - \langle \rho \rangle)^2 \rangle} \hspace{1cm} (2)$$

Here $\rho = (\rho_x, \rho_y)$ is the tilt vector, and $\langle \cdots \rangle$ denotes an average over various initial times $t_o$ in a history. We obtain an average $C(t)$ by averaging several ($\sim 10$) histories. The time is measured in units of Monte-Carlo step per site (MCS). In Fig. 3 we show $C(t)$ at different $\mu$ for $L = 24$. Similar curves have been obtained for two other system sizes, $L = 36$ and $L = 48$. The autocorrelations functions exhibit a two step-decay, which may be termed the $\beta-$ and $\alpha-$ relaxations following the standard terminology of mode-coupling theory $[11]$. Although we do not attempt a detailed analysis of the shape of these relaxation curves in this letter, several features are apparent from Fig. 3 with increasing $\mu$ the time scale of relaxation to the plateau, the plateau height, and the time scale of the decay of the plateau increase monotonically. In fact the decay time scale of the plateau $\tau$ (see inset of Fig. 3), grows exponentially and diverges at a finite $\mu$ with the divergence being well described by the Vogel-Fulcher form: $\exp(A(L)/(\mu_\ast(L) - \mu))$ for all three system sizes studied. The extrapolation of $\mu_\ast(L)$ to the infinite system indicates a divergence close to the transition point $\mu_\ast$ obtained from the equilibrium distribution.
in which the system starting from an initial state \( \rho \) evolve studying several histories (of the order of 10

\[ \begin{equation}
\text{arate on simple tilted states with the tilt pointing either}
\text{in that state for time } t \text{ and makes a transition to a new}
\text{state } \rho' \text{ in the next time interval } \delta t. \text{ From these time}
\text{histories, one can easily calculate } P_{\rho \rightarrow \rho'}, \text{ the probability that the system stayed in the state } \rho \text{ for time } t + \delta t, \text{ and}
\end{equation}

\[ P_{\rho \rightarrow \rho'} \]

\[ \text{Assuming that the tilt configurations } \{\rho\} \text{ evolve via a Markov process, the measured probabilities should have an exponential form: } P_{\rho \rightarrow \rho'} = f_1 \exp(-t/\tau_{\rho}) \text{ and } P_{\rho' \rightarrow \rho} = f_2 \exp(-t/\tau_{\rho'}), \text{ where } f_1 \text{ and } f_2 \text{ are numbers less than unity. From our extensive simulations we find that at each } \mu \text{ and for any } \rho (\text{with } \rho \neq 0) \text{ the probabilities } P_{\rho \rightarrow \rho'} \text{ and } P_{\rho' \rightarrow \rho} \text{ (for say } \rho = (\rho + 1) \text{ and } (\rho - 1) \text{) have a common exponential factor with identical decay constants } \tau_{\rho}. \text{ This evidence validates the above description in terms of the coarse-grained states } \{\rho\}. \text{ The } \rho = 0 \text{ states are an exception since we found that } P_{0 \rightarrow 0} \text{ is a stretched exponential in } t. \text{ This observation has little bearing on our current discussion, and will be taken up in the future.}

Based on the above arguments, the measurements of } P_{\rho \rightarrow \rho'} \text{ and } P_{\rho' \rightarrow \rho}; \text{ can be used directly to calculate the relaxation times } \tau_{\rho} \text{ and the transition matrix elements } W_{\rho' \rightarrow \rho} \text{ from } \rho \text{ to } \rho':

\[ \sum_{\rho' \neq \rho} W_{\rho' \rightarrow \rho} = \tau_{\rho}^{-1} \]

\[ W_{\rho' \rightarrow \rho} = \tau_{\rho}^{-1} \frac{f_2}{1 - f_1} \]  

\[ (3) \]

The variation of the relaxation time scales with the tilt \( \rho \) are shown in Fig. 2(a) for different values of \( \mu \). The most striking feature of these time scales is that \( \tau_{\rho} \) increases exponentially with \( \rho: \quad \tau_{\rho} \propto \exp(\alpha(\rho^{2\gamma})) \) with \( \gamma \) between 1/2 and 1. We will show below that the exponential increase of \( \tau_{\rho} \) arises from the jamming of non-zero winding number loops and is directly responsible for the Vogel-Fulcher divergence of the average time scale.

To explore the origin of the exponential rise of \( \tau_{\rho} \) with \( \rho \), we investigated the elements of the transition matrix \( W \) obtained from our measurements. The rates for the transition \( W_{\rho \rightarrow 1, \rho} \) and \( W_{\rho + 1, \rho} \) are plotted in Fig. 2(b) and Fig. 2(c), respectively for different \( \rho \)'s as a function of \( \mu \).
FIG. 3. We show (a) the exponential dependence of $\tau_\rho$ on $\rho$ for $\mu = 0.15, 0.175, 0.2$ and 0.22. The major contribution to the plateau timescale $\tau$ in $C(t)$ (cf Fig. 3) comes from non-simple tilts. For example, $\tau_\rho$ for $\rho = (4, 2)$ is $\approx 211$ and 660 MCS, for $\mu = 0.15$ and 0.175, respectively. (b) $W_{\rho-1, \rho}$ versus $\mu$ at $\rho = 1, 2, 3$ and 4 (from top to bottom), and (c) $W_{\rho+1, \rho}$ versus $\mu$ at $\rho = 1, 2$ and 3 (from top to bottom).

Transition rates from higher to lower tilt are well fitted by $\exp(-8\mu(2\rho-1))$. This suggests these rates to be of the form:

$$W_{\rho-1,\rho} = \Gamma_{\rho}e^{-(E_{\rho-1}-E_{\rho})}$$

(4)

The $\mu$ independent factor $\Gamma_{\rho}$, shows a negligible dependence on $\mu$ but a strong, exponential dependence on the tilt $\rho$. The origin of $\Gamma(\rho)$ can be traced back to jamming caused by the system spanning loops in a tilted state. These loops are meandering objects, and their lengths scale as $L^{3/2}$, thus squeezing in an extra loop in order to increase the tilt is associated with straightening out the existing ones. Thus the transition to higher tilt states are dramatically suppressed with increasing $\rho$ and lead to an exponential increase of $\tau_\rho$. Using Eqs. 3 and 4, the time scales can be expressed as:

$$\tau_\rho = \frac{1}{W_{\rho+1,\rho} + W_{\rho-1,\rho}} = \frac{1/\Gamma_{\rho}}{\Gamma(\rho) + e^{-(E_{\rho-1}-E_{\rho})}}$$

(6)

The $\rho$-dependent blocking factor in the denominator of Eq. 4 cannot be scaled away and the exponential suppression of the downhill transitions, reflected in $\Gamma(\rho) \ll \exp(-(E_{\rho-1}-E_{\rho})) < 1$ leads to a $\tau_\rho$ being dominated by the exponential energy cost of decreasing the tilt.

e. Theory of Vogel-Fulcher divergence: We have established that the relaxation times $\tau_\rho$ grow exponentially with $\rho$ because of barriers arising from the spatial constraints imposed by the system-spanning loops. In this paragraph we discuss how the shape of $C(t)$ and the Vogel-Fulcher type divergence of $\tau$ can be related to the $\tau_\rho$. We have good numerical evidence that the time dependence of $C(t)$ is well approximated by the form:

$$C(t) \approx \frac{\sum_\rho e^{-t/\tau_\rho} P_{eq}(\rho)}{\sum_\rho P_{eq}(\rho)}$$

(7)

This form of $C(t)$ is based on the approximation that the system is perfectly correlated as long as it stays in a state with a given tilt and decorrelates completely as it leaves this state. The probability of staying in a tilt $\rho$ for a time $t$ is measured by $e^{-t/\tau_\rho}$ and $P_{eq}(\rho)$ measures the equilibrium probability of the tilt $\rho$. The above model of $C(t)$ is identical to that of the trap model of glasses.

Since $\tau_\rho$ grows exponentially with the tilt $\sim \exp(\alpha \rho^2)$, the plateau timescale in $C(t)$ is dominated by the $\tau_\rho$ corresponding to the maximum accessible tilt, $\rho_{max}$, as determined by the width of the distribution $P_{eq}(\rho)$. As the transition to the tilted state is approached, the fluctuations of $\rho$ increase leading to a power-law divergence of $\langle \rho^2 \rangle$ and $\rho_{max}$ and an exponential divergence (Vogel-Fulcher) of the plateau timescale, $\tau$.

In summary, we find that a lattice model with frustration and associated extended structures exhibits a trap dominated dynamics arising due to jamming. A phase transition involving these structures then naturally leads to an exponential divergence of timescales.

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