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► **To cite this version:**

Claudio Chamon, Leticia F Cugliandolo. A sigma model approach to glassy dynamics. *Pramana - Journal of Physics*, 2005, 64, pp.1075. hal-00170296

HAL Id: hal-00170296

<https://hal.science/hal-00170296>

Submitted on 14 Sep 2007

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A sigma-model approach to glassy dynamics

Claudio Chamon (1) and Leticia F. Cugliandolo (2)

(1) Department of Physics, Boston University, Boston, MA 02215, USA

(2) Laboratoire de Physique Théorique et Hautes Energies, Jussieu, 4 Place Jussieu
75252 Paris Cedex 05, France

Abstract. In this contribution we review recent progress in understanding fluctuations in the aging process of macroscopic systems, and we propose further tests of these ideas. We discuss how the emergence of a symmetry in aging systems, global time-reparametrization invariance, could be responsible for the observed ‘universal’ behavior of local and mesoscopic non-equilibrium fluctuations. We discuss (i) the two-time scaling and functional form of the distribution of local correlations and responses; (ii) the scaling of multi-time correlations and susceptibilities; (iii) how the above can be derived from a random surface effective action; (iv) the behavior of a diverging two-time dependent correlation length; (v) how these ideas apply to off-lattice particle systems.

1. INTRODUCTION

In recent years much effort has been devoted to the study of the dynamics of glassy systems. Even though structural glasses consist of molecules moving in a finite dimensional volume, rather than spins interacting via random exchanges on a complete (hyper) graph, disordered spin models yield a gross description of many important features of the structural glass phenomenology (see [1] for review articles). In particular, they capture the slow non-equilibrium dynamics characterized by aging macroscopic observables below T_g [2, 3].

Very recently, a number of experiments have shown the appearance of mesoscopic dynamic regions in supercooled liquids and glasses that have distinctively different dynamics from the bulk [4, 5, 6, 7, 8]. These regions are referred to as dynamic heterogeneities and have also been identified in numerical simulations [9].

In order to understand these fluctuations one must formulate a theory that goes beyond the mean-field approximation. Recently, we presented a theoretical framework to understand aging which is based on the emergence of a symmetry, *global time reparametrization invariance* (RpG), at long time scales [10, 11, 12, 13]. The *global* RpG invariance suggests a description of the low energy physics of the glassy phase with slowly varying spatially inhomogeneous time reparametrizations $t \rightarrow h_r(t)$. Comparing with the $O(N)$ non-linear sigma model [14], *global* time-reparametrizations are analogous to uniform spin rotations while *local* time reparametrizations describe the spin waves (fluctuations on the uniform solution). An important feature of this scenario is that a critical-like dynamical two-time dependent correlation length develops.

This framework allowed us to predict several properties of local dynamic fluctuations which we tested against simulations of the Edwards-Anderson (EA) spin-glass [11, 12] and several kinetically facilitated spin models with trivial non-disordered static interactions [13]. We expect that the results from our analysis carry over to any system for which this symmetry is realized.

In this report, we briefly highlight the main concepts in our theory and we discuss more lengthly how these ideas apply to off-lattice particle systems; the diverging correlation length; the scaling of multi-time correlations and susceptibilities.

2. Reparametrization invariance

Local fluctuations in a lattice model can be probed by studying

$$C_r^o(t, t_w) \equiv \frac{1}{V_r} \sum_{i \in V_r} O_i(t) O_i(t_w) - \frac{1}{V_r} \sum_{i \in V_r} O_i(t) \frac{1}{V_r} \sum_{j \in V_r} O_j(t_w). \quad (1)$$

The subindex i labels the vertices on the lattice, $O_i(t)$ is a site and time-dependent observable and $V_r = \ell^d$ is a coarse-graining volume centered at the position r . It might be convenient to replace $O_i(t)$ by $\overline{O}_i(t)$ where the overline indicates a coarse-graining in time over a time-window centered on t . This is a local connected function that evolves from a time-dependent value at equal times to zero at diverging time separations. Bulk

(or global) correlations are obtained by setting $\ell = L$, where L is the system size. When needed, we can normalize the two-time local correlation at equal times.

Correlations that are monotonic functions of the two times take the form

$$C(t, t_w) = f\left(\frac{k(t_w)}{k(t)}\right), \quad t \geq t_w, \quad (2)$$

with $k(t)$ ($f(x)$) a monotonically increasing (decreasing) function within each ‘correlation scale’ [3]. The relaxation is given by $\partial_t C(t, t_w) = -g(C) d_t k(t)/k(t)$ with $g = x d_x f(x)$ and $x = k(t)/k(t_w)$. If $k(t) \propto e^{-t/\tau}$ one recovers a stationary scaling and $\partial_t C$ is a finite function of C itself. For any other choice of k , there is an explicit dependence on t_w (*aging*) and the variation of the correlation gets slower as time increases. For example, if $k(t) = t^a$ (as in a system undergoing domain-growth), $\partial_t C \propto t^{-1}$. Slow decays scalings as in (2) have been observed in calculations, simulations and experiments. In the following we assume, for concreteness, that the model has a single slow scale.

Mean-field disordered models are particularly interesting since the exact dynamic equations for the global correlation, $C(t, t_w)$, and linear susceptibility to a uniform field constantly applied between t_w and t , $\chi(t, t_w)$, can be derived in the thermodynamic limit. The evolution after a long waiting-time is such that a *separation of time-scales* develops, with a first relaxation in which C decays in a time-translational invariant manner ($k(t) \propto e^{-t/\tau}$) from 1 to a plateau value q_{ea} , and a second slow aging relaxation from q_{ea} to 0 with another function $k(t)$ (this can occur in a single correlation scale as in the p spin spherical model [2] or in a sequence of them as in the Sherrington-Kirkpatrick model [3]). Figure 1-left sketches the decay of a correlation for t_w fixed as a function of $t - t_w$. The three curves correspond to different choices of $k(t)$ in the aging regime.

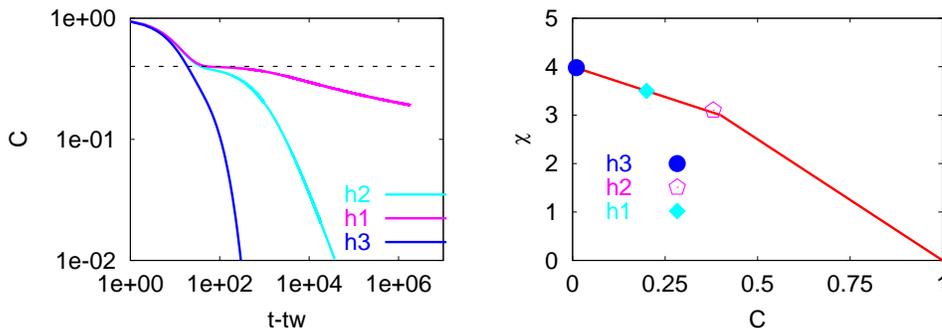


Figure 1. Left: sketch of the decay of the correlation for three choices of the scaling function $h_1(t) = t/t_0$, $h_2(t) = \ln(t/t_0)$ and $h_3(t) = e^{\ln^\alpha(t/t_0)}$. Right: the relation between the integrated response against the correlation. With solid line, the parametric plot for fixed and long t_w , using t as a parameter that increases from t_w at $C = 1$ to ∞ at $C = 0$. With symbols, the three couples $(C_j(t, t_w), \chi_j(t, t_w))$ for the same t_w , a fixed value of t and $h_j(t)$ behaving as in the left panel.

The separation of time-scales manifests in the structure of the dynamic equations. These can be separately analyzed in the $C \geq q_{ea}$ regime, that is realized at short time-

differences, and the $C < q_{ea}$ regime, that corresponds to long time-differences. The equations for $C < q_{ea}$ become invariant under *time-reparametrizations*

$$t \rightarrow h(t) , \quad \tilde{C}(t, t_w) = C(h(t), h(t_w)) , \quad \tilde{\chi}(t, t_w) = \chi(h(t), h(t_w)) , \quad (3)$$

in the asymptotic limit of diverging waiting-times [2, 3, 15, 16, 17, 18]. This also occurs in the dynamic equations arising from any resummation scheme applied to a glassy model [19].

The mechanism discussed above can be illustrated with an example. The integro-differential equation

$$\frac{\partial f(x, y)}{\partial x} = -G[f(x, y)] + \int_0^x dx' f(x, x') \frac{\partial f(x', y)}{\partial x'} \quad x \geq y , \quad (4)$$

with the ‘border’ condition $f(x, x) = 1$ and G some well-behaved function has a unique solution that can be constructed numerically. If the derivative can be dropped when $x \gg y$ the remaining (approximate) equation admits a family of solutions. Indeed, if $f_{sol}(x, y)$ is a solution, $f_{sol}(h(x), h(y))$ for *any* monotonic h is a solution as well. This can be easily seen by noting that the integral term transforms as $\int_0^x dx' f(x, x') \partial_{x'} f(x', y) = \int_0^h dh' f(h, h') \partial_{h'} f(h', h'')$, where $h \equiv h(x)$, $h' \equiv h(x')$, $h'' \equiv h(y)$, while the term $G[f(x, y)]$ is naturally invariant under this change.

Which are the symmetry properties of the *action* of a *finite dimensional* model? We addressed this question in [10] where we studied the d -dimensional EA spin-glass. Assuming causality, unitarity and a separation of time-scales we found that the disordered averaged generating functional (evaluated with no sources) can be written as

$$\overline{Z_{dyn}} = \int \mathcal{D}Q_r^{ab}(t, t_w) e^{-S_{inv}[Q_r^{ab}] - S_{non-inv}[Q_r^{ab}]} . \quad (5)$$

The expectation value of the ‘two-time dependent local fields’ Q_r^{ab} with $a, b = 1, 2$ encode the local correlation and the advanced and retarded response functions (the fourth component is zero if causality is respected). The total action is the sum of a term, S_{inv} , that is invariant under the *global* time-reparametrization, $t \rightarrow h(t)$ with $h(t)$ a monotonic function, that acts on the *local* fields as

$$\tilde{Q}_r^{ab}(t, t_w) = (d_t h(t))^a (d_{t_w} h(t_w))^b Q_r^{ab}(h(t), h(t_w)) , \quad (6)$$

and a second term, $S_{non-inv}$, that is not. The latter symmetry breaking term describes the dynamics at short-time and short time-differences and it is responsible for selecting a particular parametrization, $k(t)$, with which the global C decays in its slow regime (if $S_{non-inv}$ were absent C would be a constant). However, $S_{non-inv}$ becomes less and less important (scales down to zero) when observing longer times and time-differences, for which the (approximate) symmetry is better and better realized.

The dynamics of this problem parallels the statics of the Heisenberg ferromagnet:

$$H = \int d^d r \left[(\nabla \vec{m}(\vec{r}))^2 + g(m^2(\vec{r}) - 1)^2 + \vec{h}(\vec{r}) \cdot \vec{m}_0(\vec{r}) \right] . \quad (7)$$

The first two terms are invariant under a global rotation of the field $\vec{m}(\vec{r})$ (the equivalent of the global time-reparametrization). The last term breaks this symmetry and selects

a particular direction $\vec{m}_0(\vec{r})$ (the scaling $k(t)$ of the global correlation). If the strength of the field \vec{h} is diminished, temperature induces *longitudinal* fluctuations: the direction of the magnetization is not fixed everywhere in space but it can vary in a smooth manner generating spin-waves (the first term penalizes rapid spatial variation of the magnetization direction). Note, however, that while the field-term is relevant in the RG sense for the Heisenberg ferromagnet, the corresponding terms in the dynamic problem are irrelevant. The second term in (7) is a soft constraint on the magnitude of the magnetization and penalizes *transverse* fluctuations. (See Fig. 2-right for a sketch of the local fluctuations allowed).

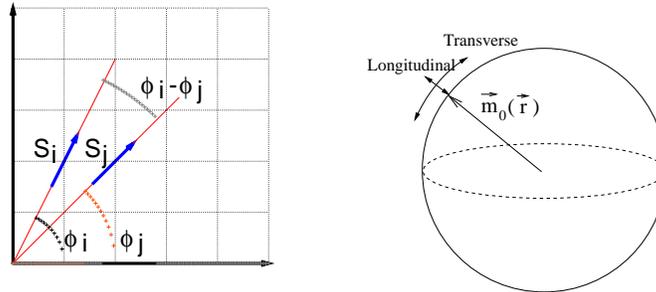


Figure 2. Left: the Heisenberg ferromagnet on a 3d lattice. Right: the 3d vector describing the magnetization on a spatial point in space. The longitudinal and transverse fluctuations are indicated with arrows.

Let us now introduce the main consequences of the (approximate) R p G.

2.1. Two-time scaling

The slow part of the coarse-grained *local* correlations and susceptibilities should scale as

$$C_r(t, t_w) \sim f_C \left(\frac{h_r(t_w)}{h_r(t)} \right), \quad \chi_r(t, t_w) \sim f_\chi \left(\frac{h_r(t_w)}{h_r(t)} \right), \quad (8)$$

with f_C and f_χ the same functions describing the global correlation and susceptibility, respectively, and the same function $h_r(t)$ scaling the two-time correlation and susceptibility on each site r [10, 11, 12]. Figure 1-left sketches the behavior of three local correlations.

2.2. Multi-time scaling

In general multi-time correlations are not trivially related to the two-time ones. Let us discuss the time-dependence of the coarse-grained connected four-time correlation

$$C_r(t_1, t_2, t_3, t_4) \equiv \frac{1}{V_r} \sum_{i \in V_r} O_i(t_1) O_i(t_2) O_i(t_3) O_i(t_4) - \sum_{\text{pairs}} \frac{1}{V_r} \sum_{i \in V_r} O_i(t_k) O_i(t_l) \frac{1}{V_r} \sum_{i \in V_r} O_i(t_m) O_i(t_n) + \prod_{k=1}^4 \frac{1}{V_r} \sum_{i \in V_r} O_i(t_k) \quad (9)$$

as an example. If this function is monotonic with respect to all times, one proposes [22] that, if the two-point correlations scales as in (2) for all pairs (t_i, t_j) with $i, j = 1, 2, 3, 4$, the four-time correlation should behave as

$$C_r(t_1, t_2, t_3, t_4) = f_{C^4} \left(\frac{k_r(t_1)}{k_r(t_2)}, \frac{k_r(t_2)}{k_r(t_3)}, \frac{k_r(t_3)}{k_r(t_4)} \right) \quad (10)$$

with the same external function f_{C^4} for all r .

2.3. Local fluctuation-dissipation relation

The asymptotic relation between the global correlation and susceptibility

$$\lim_{t_w \rightarrow \infty, C(t, t_w) = C} \chi(t, t_w) = \hat{\chi}(C) \quad (11)$$

was first obtained in mean-field disordered systems [2, 3, 17] and later observed in simulations of many realistic models. The solid line in the right-panel in Fig. 1 sketches the function $\hat{\chi}(C)$ for a system with two correlation scales and demonstrates that the FDT is broken. $-(d_C \hat{\chi}(C))^{-1}$ defines an effective temperature [20].

The scaling in (8) implies that in a parametric construction the local correlation and susceptibility should fall on the master curve for the global quantities but can be advanced or retarded with respect to the global value leading to heterogeneous aging with some regions younger (older) than the global average. This is the constraint in the σ -model construction. and it is sketched in Fig. 1-right for the three sites displayed in the left panel. In Fig. 3 we show the joint PDF of local correlations and susceptibilities of the EA spin-glass; the accord with the analytic prediction is very satisfactory [11, 12].

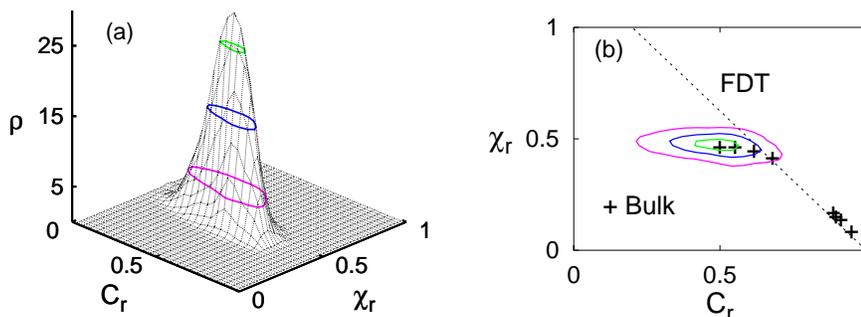


Figure 3. (a) The joint PDF $\rho(C_r, \chi_r)$ at two times (t_w, t) such that the global correlation is $C(t, t_w) = 0.7 < q_{ea}$ in the 3d EA model. (b) Projection of three contour levels. The crosses are the parametric construction $\hat{\chi}(C)$ for several values of the total time t larger than t_w . The dotted straight line is FDT at the working temperature T .

2.4. Two-time correlation length

The local correlation C_r depends on the linear length ℓ used to coarse-grain. Which values of ℓ should be used? Before addressing this question let us recall our definition

of a two-time dependent correlation length $\xi(t, t_w)$ [12, 23]:

$$A(\Delta \equiv |\vec{r}_i - \vec{r}_j|; t, t_w) \equiv \frac{1}{V} \sum_{i=1}^N O_i(t) O_i(t_w) O_j(t) O_j(t_w), \quad (12)$$

$$B(\Delta, t, t_w) \equiv \frac{A(\Delta; t, t_w) - A(\Delta \rightarrow \infty; t, t_w)}{A(\Delta = 0; t, t_w) - A(\Delta \rightarrow \infty; t, t_w)} \approx e^{-\Delta/\xi(t, t_w)} \quad (13)$$

(we omitted a possibly present algebraic factor). We used a notation that is adapted to a lattice problem; the generalization to an off-lattice model can be easily done following the discussion in 3. We expect $\xi(t, t_w)$ to diverge in the long waiting-time and time-difference limit due to the generation of the zero mode. The numerical results for the $3d$ EA model are compatible with this expectation although the actual values of ξ reached are pretty small (of the order of 5 lattice spacings).

Thus, if we are interested in studying the asymptotic non-equilibrium scaling limit ℓ should be such that $a \ll \ell \ll \xi(t, t_w)$ with a the lattice spacing (or typical interparticle distance). The first condition leads to smooth local correlations. The second one ensures that we are not erasing all fluctuations with the coarse-graining. We thus expect to find similar fluctuations using finite size systems and examining the behavior of the mesoscopic run-to-run fluctuations of the global correlations [24].

The PDFs of local correlations should crossover from a non-trivial form to a simple Gaussian when ℓ goes through the value ξ ; the analysis of the ℓ -dependent PDFs thus provides an independent way to determine $\xi(t, t_w)$.

Note that the fluctuations of the multi-time correlations (9) can be used to derive other correlation lengths. It would be interesting to check if all these behave in the same manner or not.

2.5. Effective action

One can now attempt to propose an effective action for the local aging fluctuations when $a \ll \ell \ll \xi$.

Our claim is that the external function f_C and f_χ are the same for all coarse-grained centers in the sample, while all spatial fluctuations are encoded in the internal function h_r . The reason for this proposal is that the *global* reparametrization invariance in time of the dynamic action in this two-time regime leads to low action excitations (Goldstone modes) for smoothly varying *spatial* fluctuations in the reparametrization of time, but not in the external form of the correlations. As in a sigma model, the external functions f_C and f_χ fix the manifold of states, and the local time reparametrizations correspond to fluctuations restricted to this fixed manifold of states [12].

As in the σ -model approach to an interacting system in which we have identified a relevant variable and a relevant symmetry, we propose an effective action for the relevant degree of freedom that quantifies the fluctuations about the globally symmetric result. The philosophy is the same as the one followed when describing spin-wave excitations in a Heisenberg ferromagnet with a quadratic action that depends on the angular variables only.

The scaling form in (8) can be written in an equivalent form by defining $\phi_r(t) \equiv \ln h_r(t)$:

$$C_r(t, t_w) \sim f_C \left(e^{-[\phi_r(t) - \phi_r(t_w)]} \right) = f_C \left(e^{-\int_{t_w}^t dt' \dot{\phi}_r(t')} \right) \equiv f_C \left(e^{-\Delta\phi_r|_{t_w}^t} \right). \quad (14)$$

After parametrizing the correlation in this way, the relevant field is the function $\phi_r(t)$. The action governing the dynamics of $\phi_r(t)$ depends on the details of the particular problem. However, we can greatly restrict the form of the possible actions by simply using the constraints due to the symmetries. These are the following. The action must be invariant under a global time reparametrization $t \rightarrow s(t)$. If our interest is in short-ranged problems, the action must be written using local terms. The action can thus contain products evaluated at a single time and point in space of terms such as $\phi_r(t)$, $\dot{\phi}_r(t)$, $\nabla\phi_r(t)$, $\nabla\dot{\phi}_r(t)$, and similar derivatives. The scaling form in (14) is invariant under $\phi_r(t) \rightarrow \phi_r(t) + \Phi_r$, with Φ_r independent of time. Thus, the action must also contain this symmetry. The action must be positive definite. These requirements largely restrict the possible actions and the one with the smallest number of spatial derivatives (most relevant terms) is

$$S_{\text{eff}} = K \int d^d r \int dt (\nabla d_t \phi_r(t))^2 / d_t \phi_r(t). \quad (15)$$

where we dropped a total derivative term. Since the $d_t \phi_r$ are uncorrelated at any two different times t_1 and t_2 , $\Delta\phi_r|_{t_w}^t = \int_{t_w}^t dt' \dot{\phi}_r(t')$ is a sum of uncorrelated random variables in time. Hence, one can interpret such expression as the displacement of a random walker with position dependent velocities. Alternatively, one can think of the space-dependent differences $\Delta\phi_r|_{t_w}^t = \int_{t_w}^t dt' \dot{\phi}_r(t')$ as the net space-dependent height (labeled by t) of a stack of spatially fluctuating layers $dt' \dot{\phi}_r(t')$. The action for the fluctuating surfaces of each layer is given by (15).

The results above allow us to extract all the properties of the statistical distribution of the local correlations $C_r(t, t_w)$. It is useful to write the action using the *proper time* $s(t) = \ln h(t)$ chosen by the bulk values, and by defining a new field, $\psi_r(s)$, such that $\psi_r^2(s) = \dot{\phi}_r(s)$. One then has

$$S_{\text{eff}} = K \int d^d r \int ds (\nabla \psi_r(s))^2, \quad \Delta\phi_r|_{t_w}^t = \int_{s(t_w)}^{s(t)} ds \psi_r^2(s). \quad (16)$$

The action is one of uncorrelated Gaussian surfaces for different proper times s . Due to the Gaussian statistics of the $\psi_r(s)$, it is simple to show that connected N -point correlations of $\Delta\phi_r|_{t_w}^t$ satisfy $\langle \Delta\phi_{r_1}|_{t_w}^t \Delta\phi_{r_2}|_{t_w}^t \cdots \Delta\phi_{r_N}|_{t_w}^t \rangle_c = [s(t) - s(t_w)] \mathcal{F}(r_1, r_2, \dots, r_N)$ where the function \mathcal{F} can be obtained from Wick's theorem, summing over all graphs that visit all sites (connected) with two lines (because of ψ^2) for each vertex i corresponding to a position r_i . The reparametrized times appear only in the prefactor $\Delta s = s(t) - s(t_w)$. Therefore time dependencies are functions of Δs alone and all the PDFs of local correlations depend on times only through the value of the global correlation that acts as the natural 'clock'. The scaling of the PDFs of local

correlations is the same as the one for the global C in the multi-scale problem as well. Then,

$$\rho(C_r; t, t_w) = g(C_r; C(t, t_w)) . \quad (17)$$

We checked this hypothesis in the $3d$ EA model and in several kinetically constrained spin systems. In Fig. 4-left we show $\rho(C_r(t^{(k)}, t_w^{(k)}))$ for $t^{(k)}$ and $t_w^{(k)}$, $k = 1, \dots, n$, such that $C(t^{(k)}, t_w^{(k)}) = C$ for one of the latter [13]. The collapse on a single curve verifies our prediction.

The effective action relating the fluctuations of local correlations to random surfaces allows us to determine the form of the PDFs themselves. In [13], we showed that $g(C_r; C(t, t_w))$ can be well approximated by generalized Gumbel distributions [21]. The right panel in Fig. 4 shows the PDF of ‘local’ correlations extracted from the Gaussian random manifold model. The data in the two panels resemble strikingly. The trend to approach a Gaussian distribution at very long time-differences observed experimentally is also captured by this model.

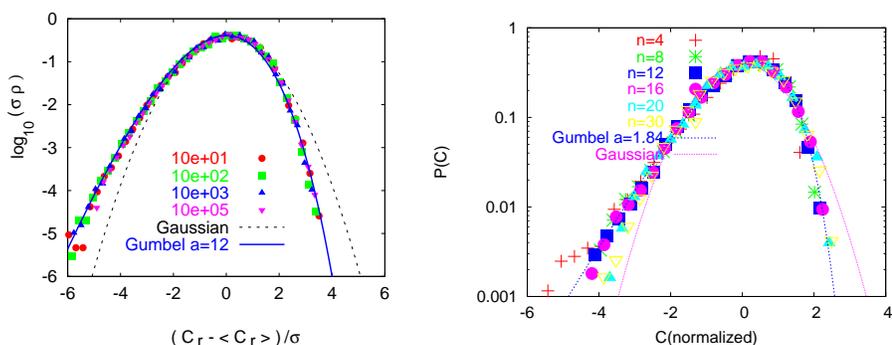


Figure 4. Left: the distribution of the coarse-grained local correlations C_r for four pairs of t and t_w such that the global correlation is equal to 0.8. The parameters given in the key determine the waiting-times in MCs. The lines indicate a Gumbel form with parameter $a = 12$ and a Gaussian PDF. Right: results from simulating a $3d$ Gaussian random manifold. The parameter n plays the role of t/t_w . The distribution slowly evolves from a Gumbel-like form to a Gaussian.

The scaling of higher-order correlations of the type in (9) can also be derived from (15).

3. Local fluctuations in off-lattice particle systems

Most glasses consist in confined ‘particles’ in interactions. Confocal microscopy is a recently developed experimental tool that allows one to follow the trajectories of these particles in colloidal systems. The PDF of particle self-displacements,

$$\Delta_i(t, t_w) \equiv |\vec{x}_i(t) - \vec{x}_i(t_w)| , \quad (18)$$

where $\vec{x}_i(t) = (x_i^1(t), \dots, x_i^d(t))$ is the position of the i -th particle at time t , have been studied with this technique [5, 6] and numerically [9].

Closer to our theoretical framework would be to study the PDFs of box-averaged displacements defined as follows. First, divide the full volume $V = L^d$ into m cells of size ℓ^d in such a way that $V = m\ell^d$. Next, compute the average displacement within the box,

$$\Delta_r(t, t_w) \equiv \frac{1}{n} \sum_{j=1}^n \Delta_j(t, t_w) \quad (19)$$

summing over the particles that were in the box at time t_w only. Note that the actual total self-displacements reached experimentally are tiny – of the order of half the radius of the particles [6]. Thus, the number of particles that leave or enter the box between t_w and t is negligible for moderate linear cell sizes.

Concerning the local responses, one can apply random fields on each particle between the waiting-time t_w and the observation time t , and then define box susceptibilities by summing over the staggered displacements of the particles that were within the box at time t_2 . Again, for weak enough perturbation and large enough linear-size of the cell, essentially no particle should leave or enter the box.

4. Conclusions

The theoretical framework in Refs. [10, 11, 12, 13] is based on a simple premise: the long time dynamics of glassy systems is governed by some effective action that is invariant under reparametrizations of time. For spin-glasses, we have shown that the emergence of this symmetry is a consequence of causality and unitarity, and a separation of time scales into fast and slow regimes [10]. In this report, we presented a summary of some of the predictions of this theory on the statistical and dynamic properties of spatial fluctuations. We also presented some new predictions that we plan to test in the future.

We wish to especially thank H. E. Castillo, P. Charbonneau, J. L. Iguain, M. P. Kennett, D. Reichman and M. Sellitto for our collaboration on the results that we discussed in this article. This work was supported in part by the NSF grants DMR-0305482 and INT-0128922 (CC), a CNRS-NSF collaboration, the ACI Jeunes Chercheurs “Algorithmes d’optimisation et systèmes désordonnés quantiques” and the Guggenheim Foundation (LFC).

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