Time reparametrization symmetry and fluctuations in glassy systems

Horacio E. Castillo — Ohio University, Athens OH

Collaborators:

Azita Parsaeian — Ohio University, Athens OH

Claudio Chamon — Boston University
Leticia F. Cugliandolo — ENS, Paris
José L. Iguain — Université de Montréal
Malcolm P. Kennett — Simon Fraser University

Supported by *NSF* and *CNRS*.

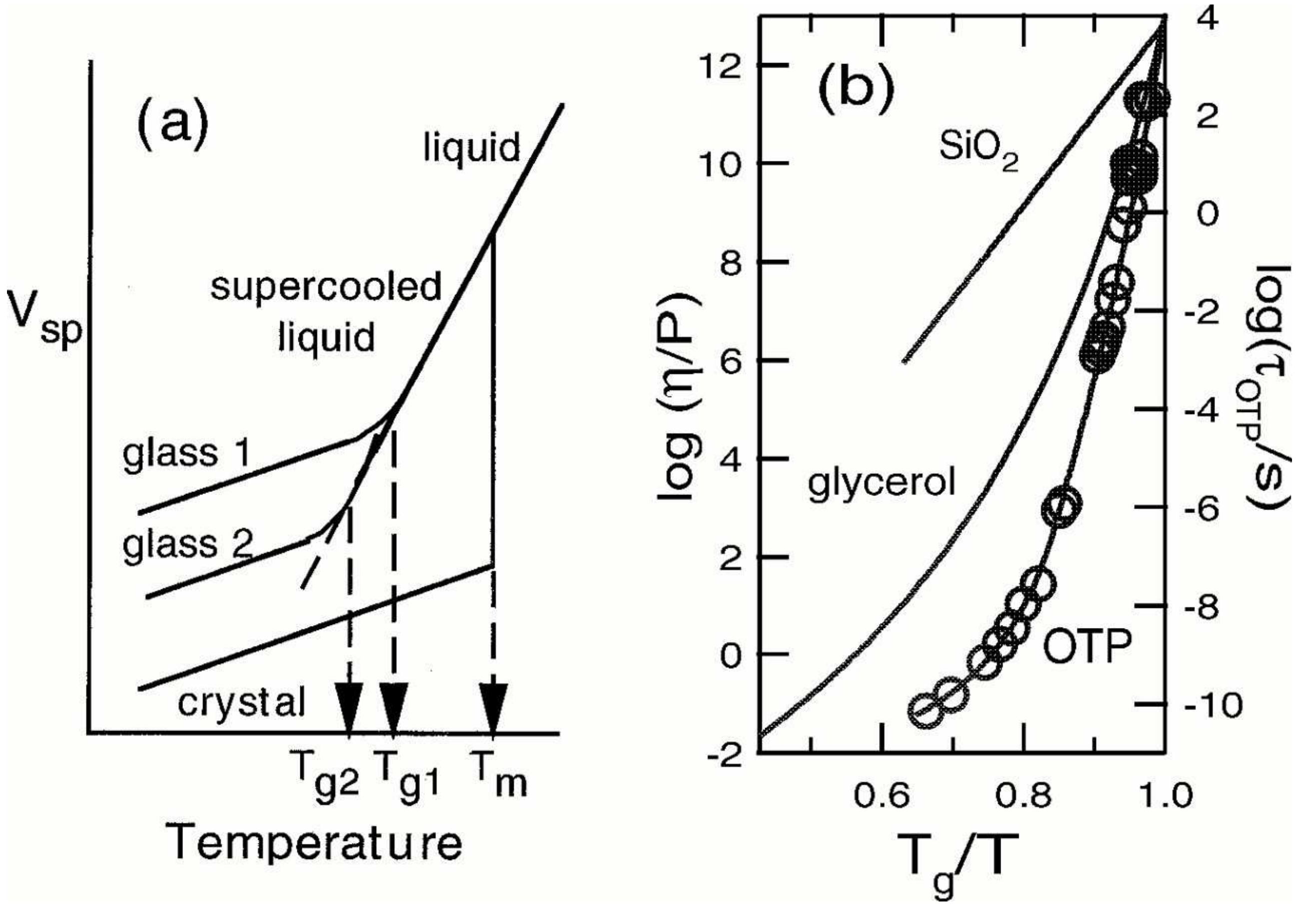
See: PRL **89**, 217201 (2002); PRL **88**, 237201 (2002); and PRB **68**, 134442 (2003)

Workshop on Stochastic Geometry and Field Theory

KITP, UCSB

Santa Barbara; CA, August 24, 2006

Slow dynamics in glasses

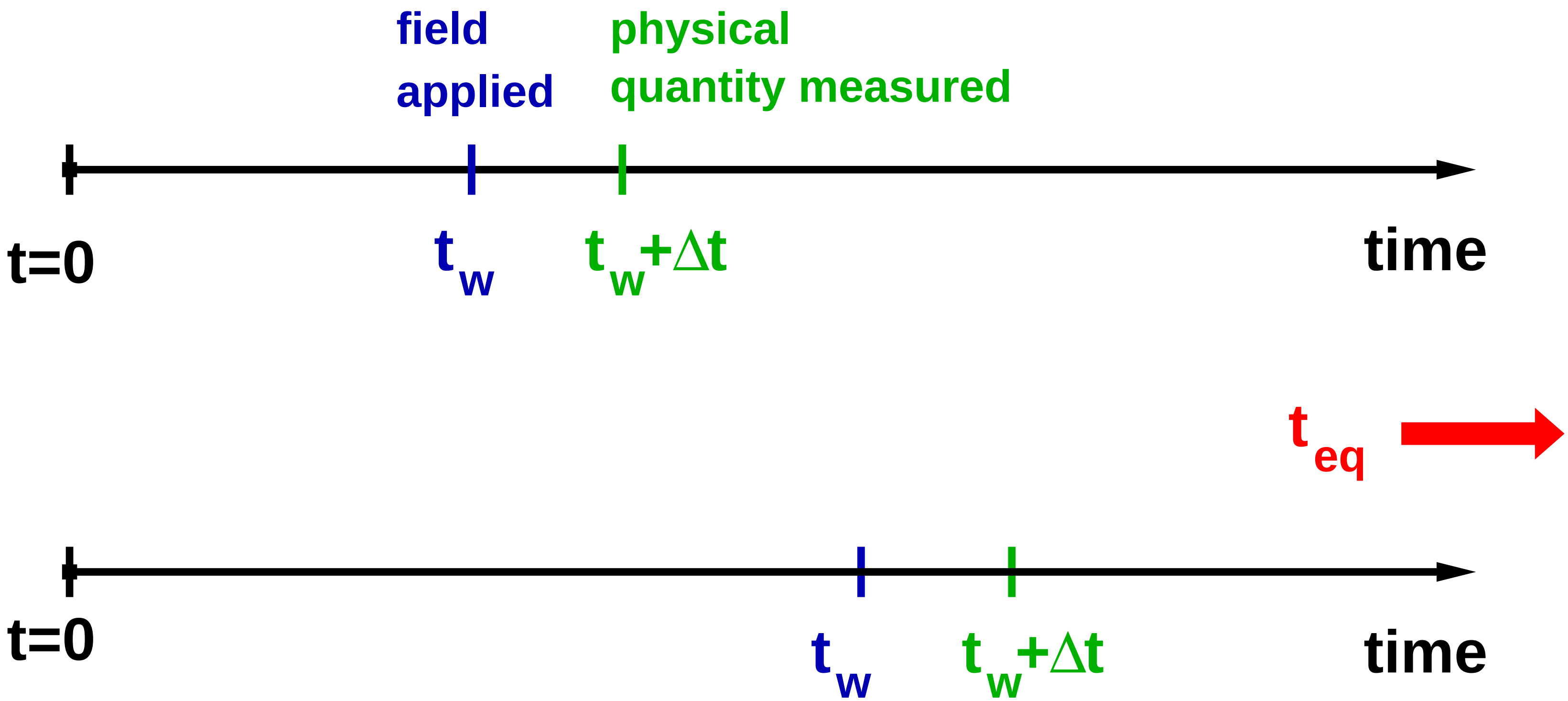


M.D.Ediger
(2000)

(a) At the glass transition, the system "falls out" of equilibrium.

(b) Viscosities and relaxation times increase dramatically as a material cools towards T_g.

Material in a glassy state

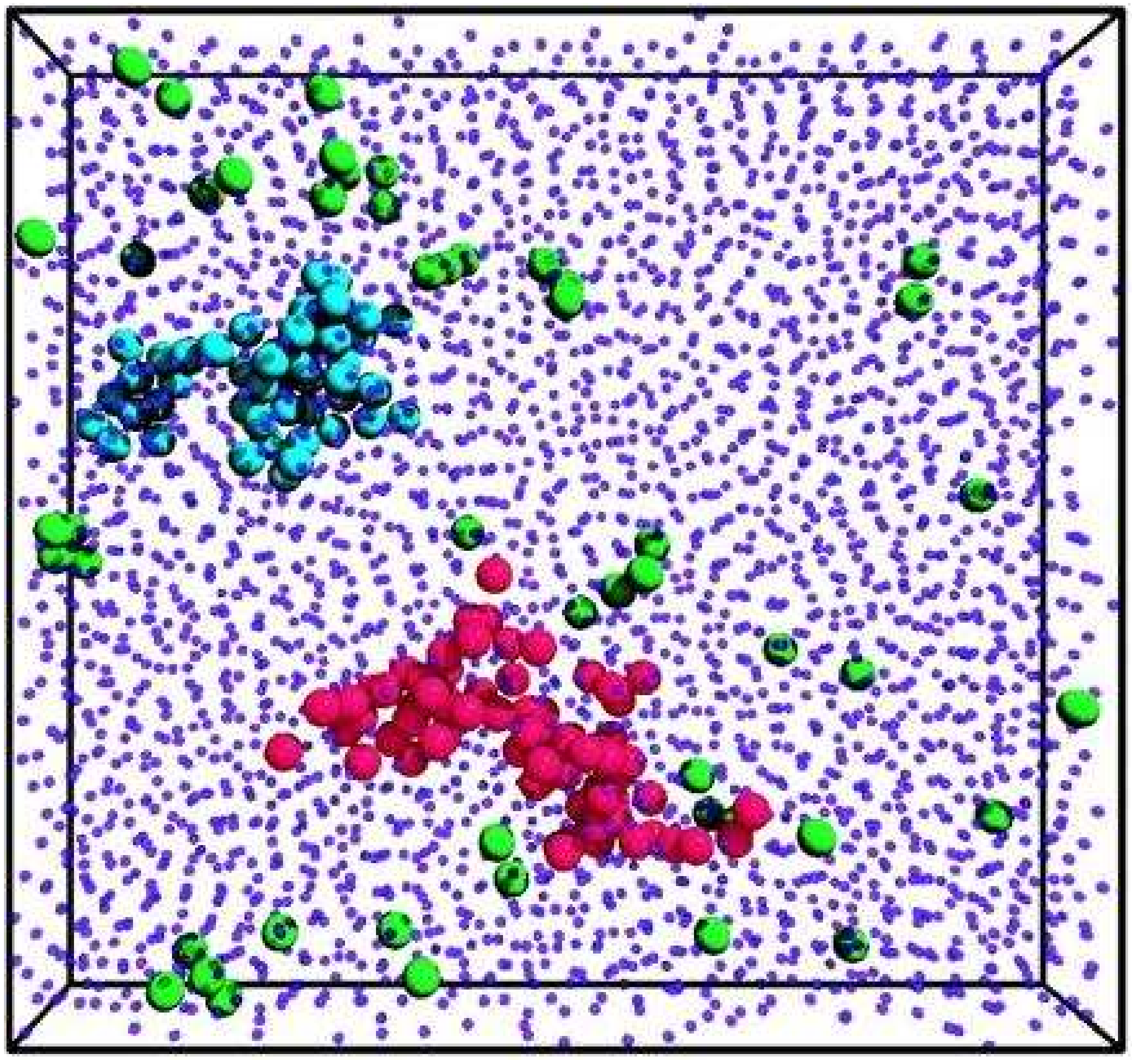


The two experiments give different results

TTI Broken: AGING !!

The Problem: Dynamical heterogeneities

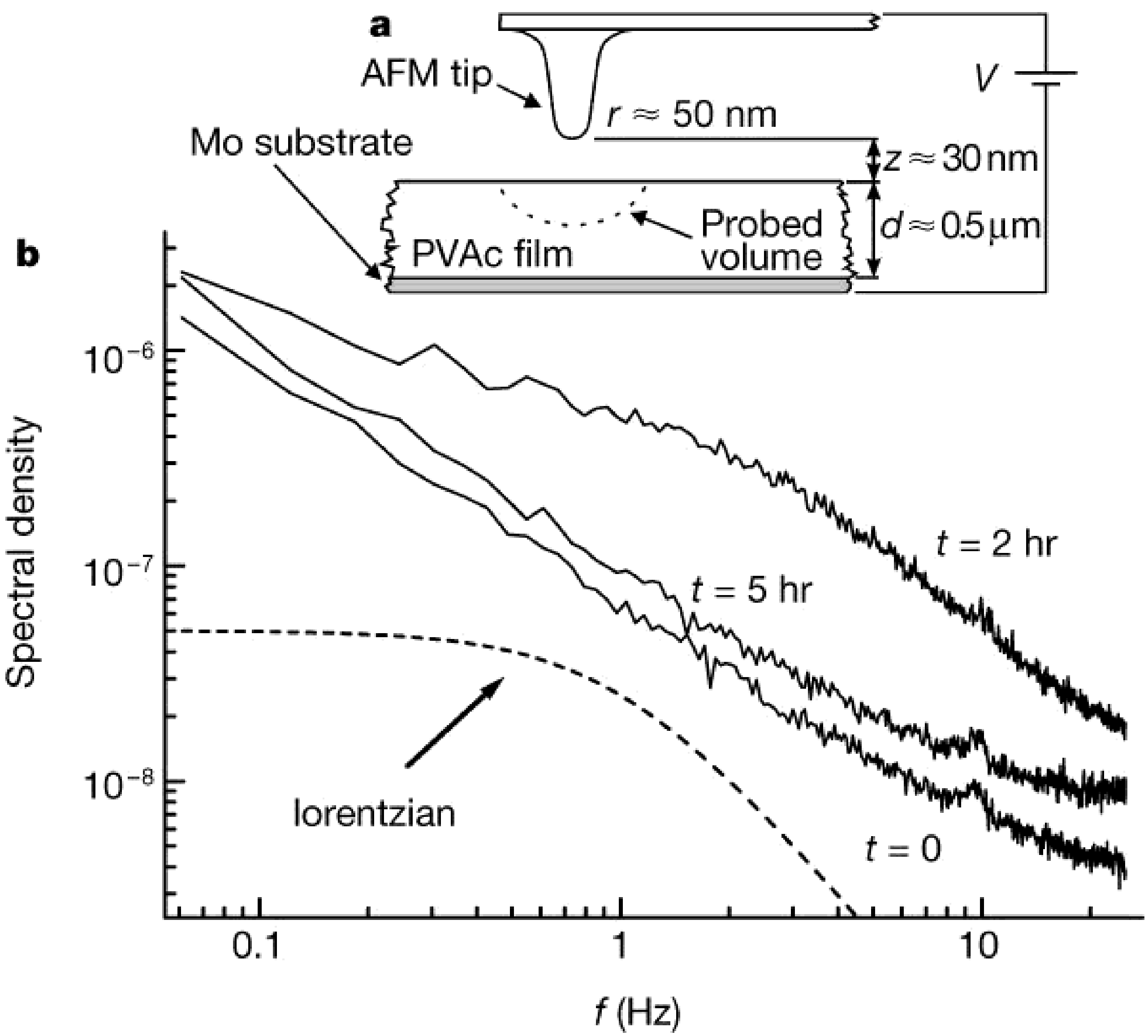
Colloid: confocal microscopy (Weeks et al., Science **287**, 627 (2000))



Supercooled liquid, the fastest 5% of the particles are highlighted

The Problem: Dynamical heterogeneities

PVAc: dielectric fluctuations (Vidal Russell & Israeloff, Nature **408**, 695 (2000))



Polymer glass, $T = T_g - 9K$, transient appearence of strongly fluctuating region under tip

Heterogeneity lifetime ≈ relaxation time

Motivation

- Experiments show spatially heterogeneous dynamics.
- We don't have a theory of spatial fluctuations in glassy dynamics

Outline

1. Experiments show that glasses are out of equilibrium: age-dependent effects ("Physical aging") and "FDT violations".
2. Symmetry under time reparametrization. Goldstone mode: space dependent ages in glassy systems.
3. Numerical evidence in models of spin glasses and structural glasses.

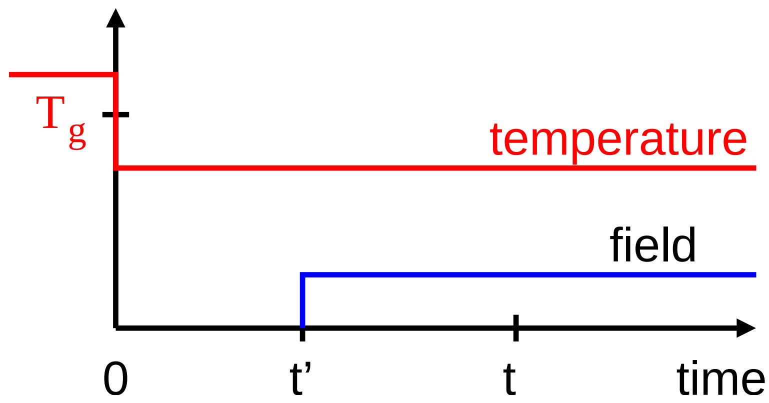
Outline

1. Experiments show that glasses are out of equilibrium: age-dependent effects ("Physical aging") and "FDT violations".

2. Symmetry under time reparametrization. Goldstone mode: space dependent ages in glassy systems.

3. Numerical evidence in models of spin glasses and structural glasses.

Fluctuation - response in spin glasses



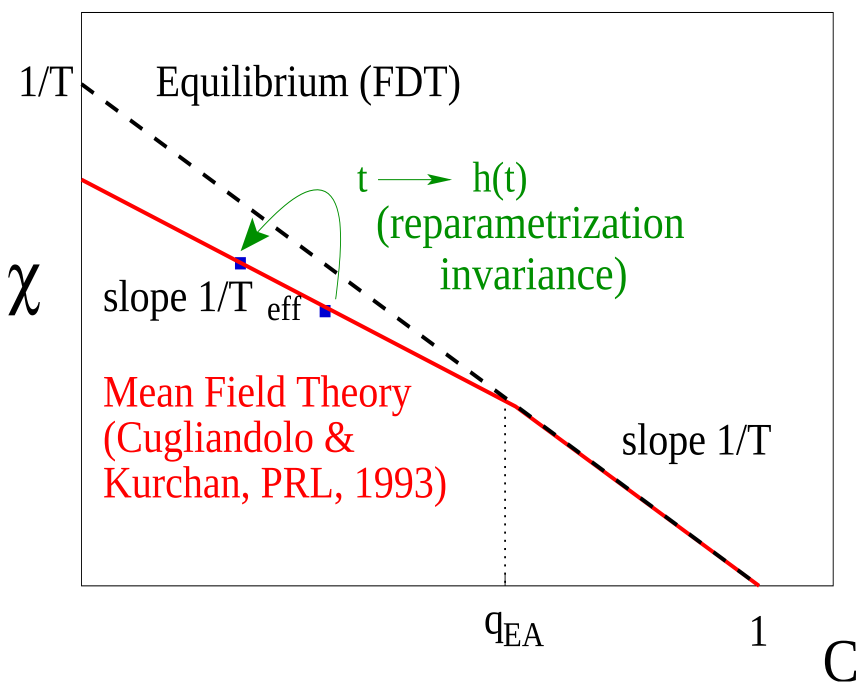
Correlation (noise)

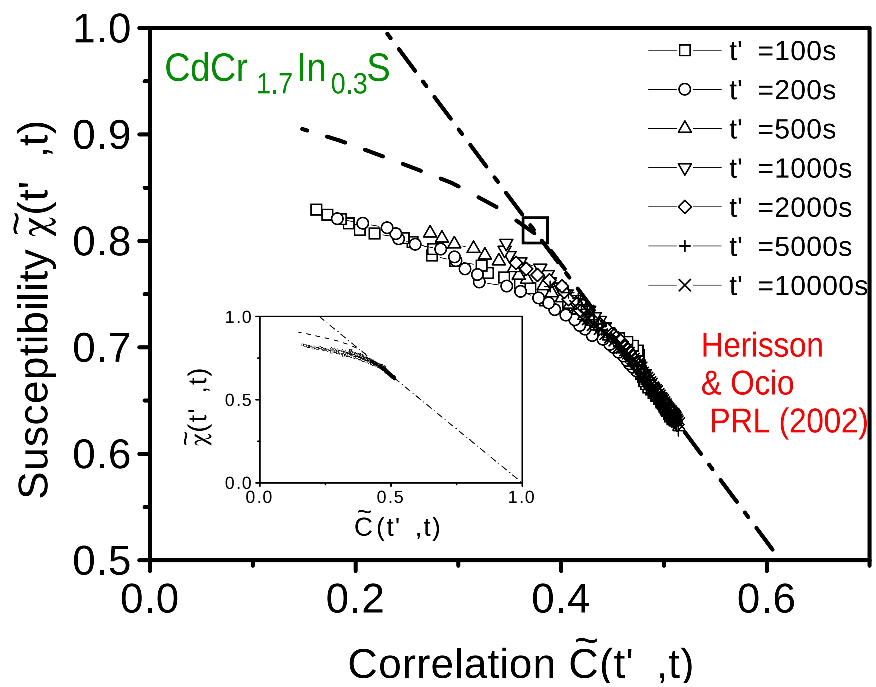
$$C_{\vec{r}}(t,t') \equiv \frac{1}{V_{\vec{r}}} \sum_{i \in V_{\vec{r}}} S_i(t) S_i(t')$$

Response (susceptibility)

$$R_{\vec{r}}(t,t') \equiv \frac{1}{V_{\vec{r}}} \sum_{i \in V_{\vec{r}}} \partial S_i(t)/\partial h_i(t')$$

$$\chi_{\vec{r}}(t,t') \equiv \int_{t'}^{t} dt'' R_{\vec{r}}(t,t'')$$





Outline

1. Experiments show that glasses are out of equilibrium: age-dependent effects ("Physical aging") and "FDT violations".

2. Symmetry under time reparametrization. Goldstone mode: space dependent ages in glassy systems.

3. Numerical evidence in models of spin glasses and structural glasses.

A toy example: Mean Field p-Spin Model

Cugliandolo and Kurchan, PRL **71**, 173 (1993)

- Dynamical equations for correlation and response ($\mu \equiv p\beta^2/2$):

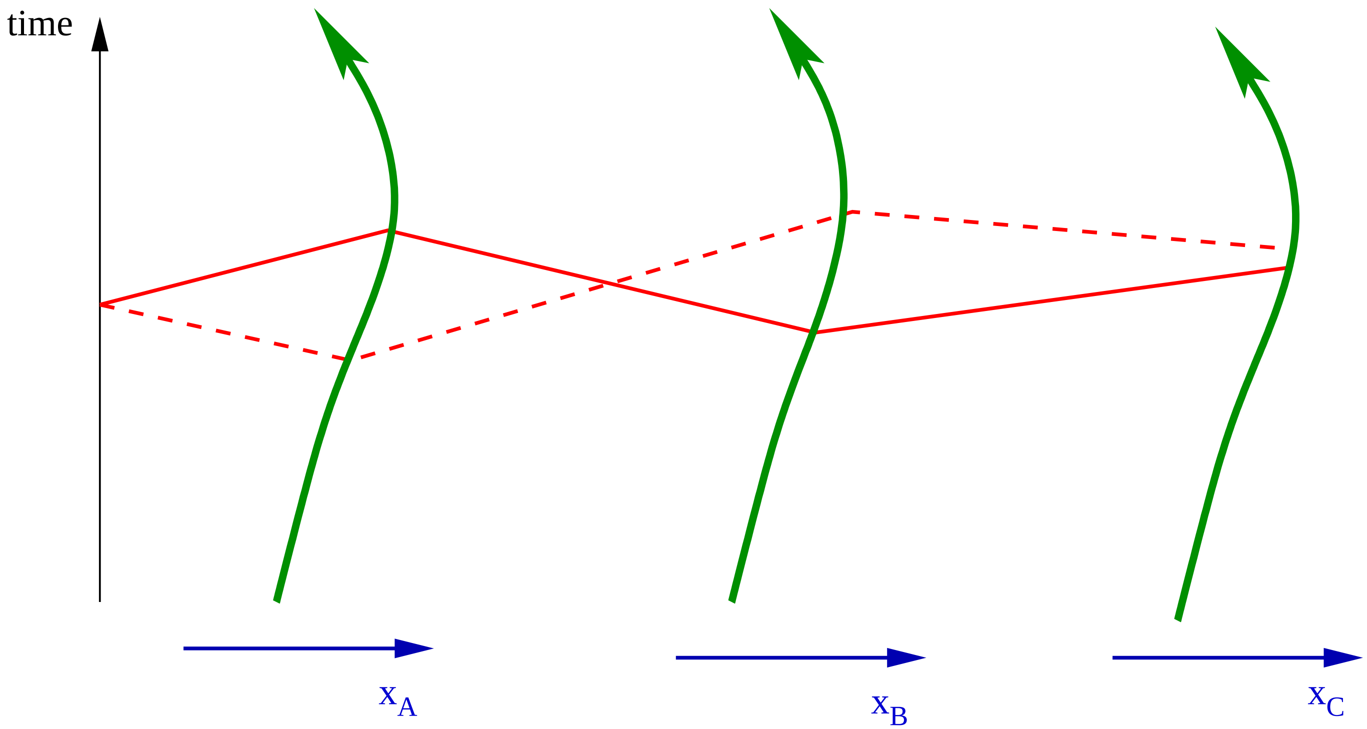
$$
\begin{aligned}
\frac{\partial C(t,t')}{\partial t} &= -\left(1 - p\beta\,\mathcal{E}(t)\right) C(t,t') + 2\,R(t',t) \\
&\quad + \mu \int_0^{t'} dt''\, C^{p-1}(t,t')\, R(t',t'') \\
&\quad + \mu\,(p-1) \int_0^{t} dt''\, R(t,t'')\, C^{p-2}(t,t'')\, C(t'',t') \\
\frac{\partial R(t,t')}{\partial t} &= -\left(1 - p\beta\,\mathcal{E}(t)\right) R(t,t') + \delta(t-t') \\
&\quad + \mu\,(p-1) \int_{t'}^{t} dt''\, R(t,t'')\, C^{p-2}(t,t'')\, R(t'',t')
\end{aligned}
$$

- Reparametrization invariance: in the limit of slow dynamics, the dynamical equations are still satisfied if $C(t,t')$ and $R(t,t')$ are replaced by:

$$
\tilde{C}(t,t') = C(h(t),h(t')) \qquad \tilde{R}(t,t') = R(h(t),h(t'))\frac{dh}{dt'}
$$

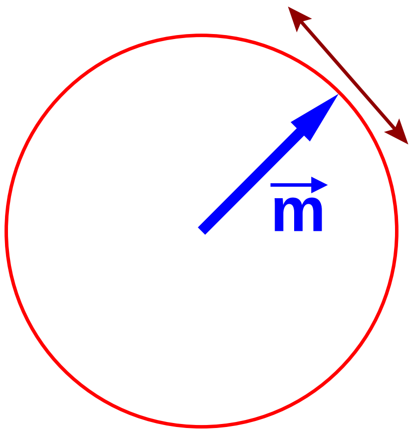
Can we understand dynamical heterogeneities?

A possible explanation: the glassy material is aging, but the ages are fluctuating in space.



Can we understand dynamical heterogeneities?

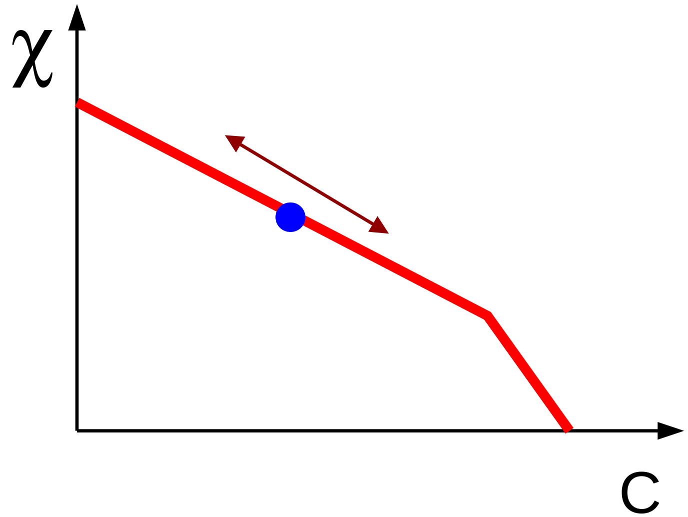
Equilibrium state of ferromagnet



Rotations $\mathcal{R}_\theta$ leave free energy $\mathcal{F}$ unchanged

Minimization of $\mathcal{F}[\vec{m}(\vec{r})]$ selects the (mean field approx.) physical magnetization

Nonquilibrium dynamics of spin glass



RG in time: reparametrizations $t \to h(t)$ leave "dynamical action" $\mathcal{S}$ unchanged

(irrelevant terms break symmetry at finite times)

(C.Chamon, M.P.Kennett, H.E.C., L.F.Cugliandolo, PRL **89**, 217201 (2002))

Minimization of $\mathcal{S}[(C_{\vec{r}}(t,t_w), \chi_{\vec{r}}(t,t_w))]$ selects the (mean field approx.) physical evolution of (C, χ)

Can we understand dynamical heterogeneities?

Equilibrium state
of ferromagnet

Fluctuations with high
probability (small $\delta\mathcal{F}$):

$$\mathcal{R}_{\theta(\vec{r})}$$

(direction of the
magnetization varies
smoothly in space)
"magnons"

Nonquilibrium dynamics
of spin glass

Fluctuations with high
probability (small $\delta\mathcal{S}$):

$$t \rightarrow h_{\vec{r}}(t)$$

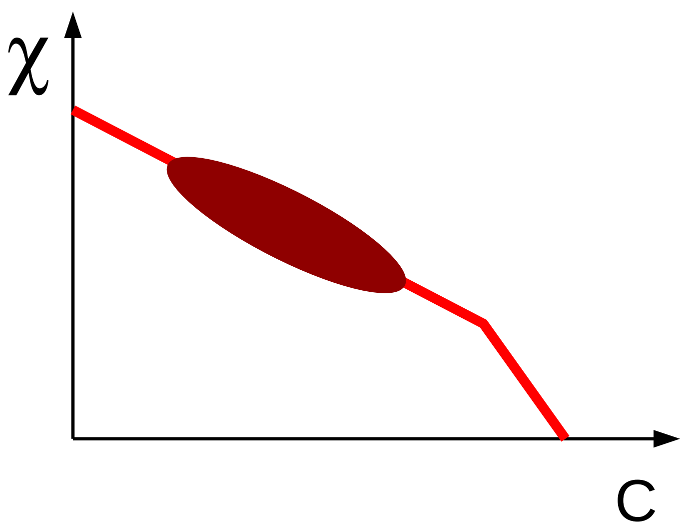
(age of the material varies
smoothly in space)

(H.E.C., C.Chamon,
L.F.Cugliandolo, M.P.Kennett,
PRL **88**, 237201 (2002))

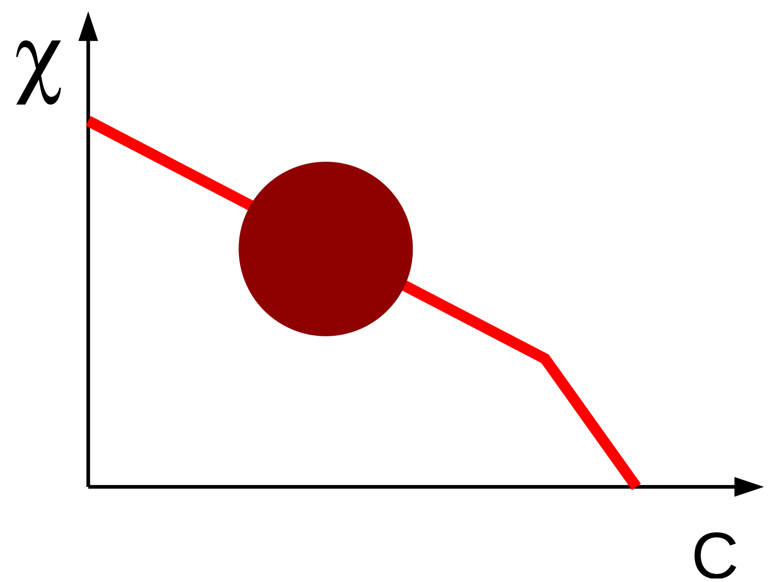
How do we test this theoretical framework?

1. Measure $C_{\vec{r}}(t, t_w)$ and $\chi_{\vec{r}}(t, t_w)$ at fixed, large (t, t_w).

2. See where the points accumulate in the (C, χ) plane.



OK!!



Doesn't work!!

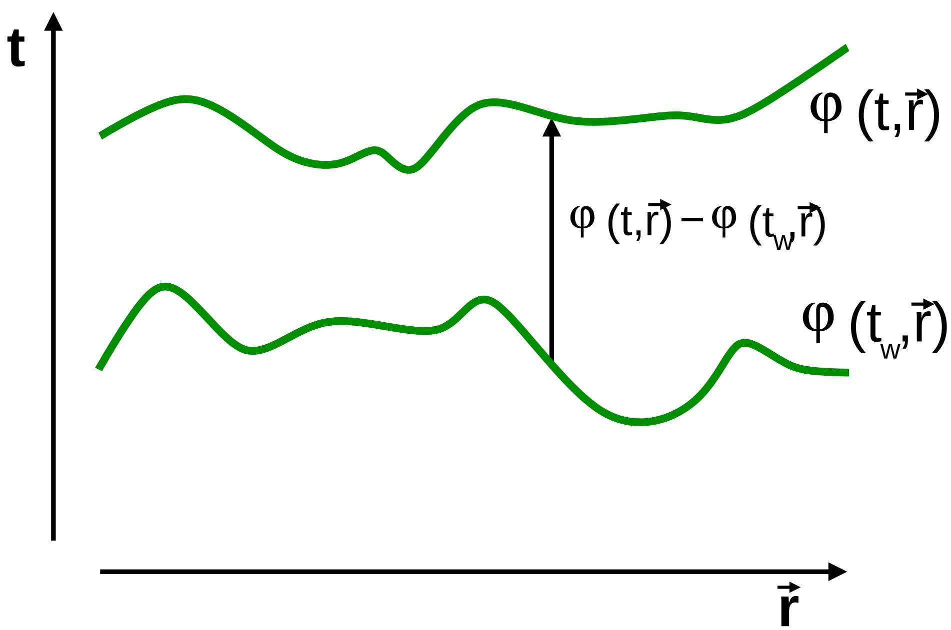
Probability distribution of local correlations: $\rho(C_{\vec{r}})$

(with C. Chamon, L. Cugliandolo, J. Iguain, and M. Kennett: PRL **88**, 237201 (2002) and PRB **68**, 134442 (2003))

If $C_0(t,t_w) \approx C_0(h(t)/h(t_w))$ (for example, $h(t) \approx t$ in 3DEA) then:

$$t \to h_{\vec{r}}(t) = \mathrm{e}^{\varphi_{\vec{r}}(t)}$$

$$C_{\vec{r}}(t,t_w) = C_0(h_{\vec{r}}(t)/h_{\vec{r}}(t_w)) = C_0(\exp(\varphi_{\vec{r}}(t) - \varphi_{\vec{r}}(t_w)))$$



- Fluctuating $\varphi_{\vec{r}}(t)$
- Time reparametrization invariance
- $\Rightarrow \varphi_{\vec{r}}(t) - \varphi_{\vec{r}}(t_w) \approx \ln\left(\frac{h(t)}{h(t_w)}\right) + \sqrt{a + b\ln\left(\frac{h(t)}{h(t_w)}\right)}\, X_r$

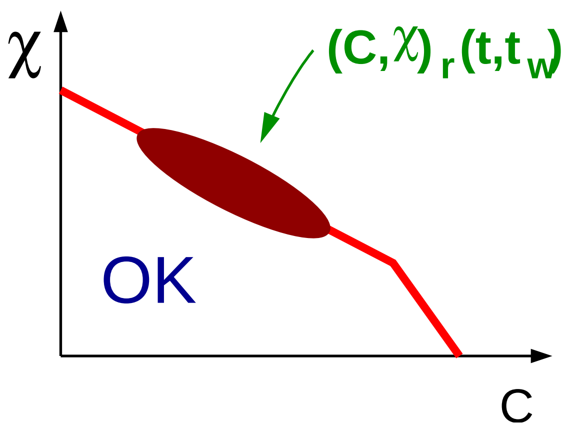
Outline

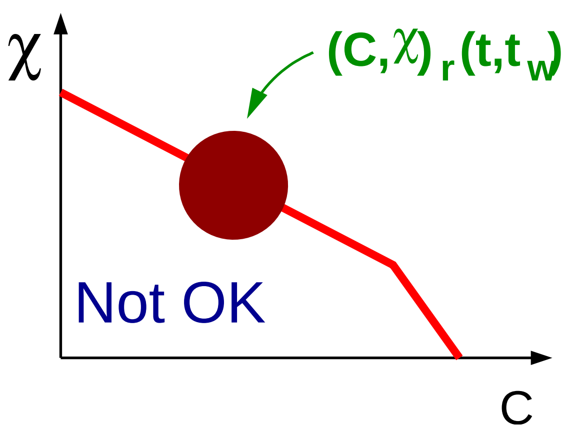
1. Experiments show that glasses are out of equilibrium: age-dependent effects ("Physical aging") and "FDT violations".

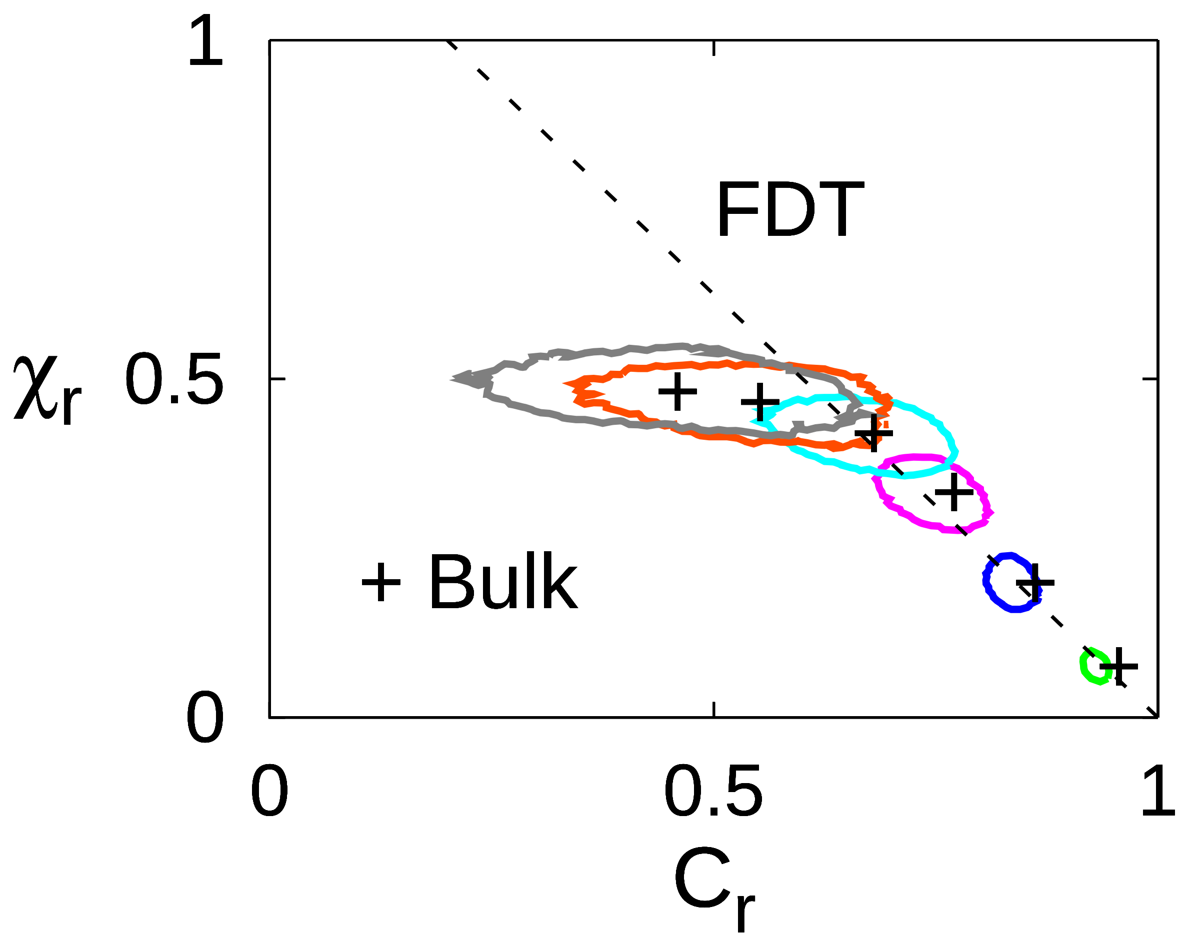
2. Symmetry under time reparametrization. Goldstone mode: space dependent ages in glassy systems.

3. Numerical evidence in models of spin glasses and structural glasses.

Testing the theoretical framework





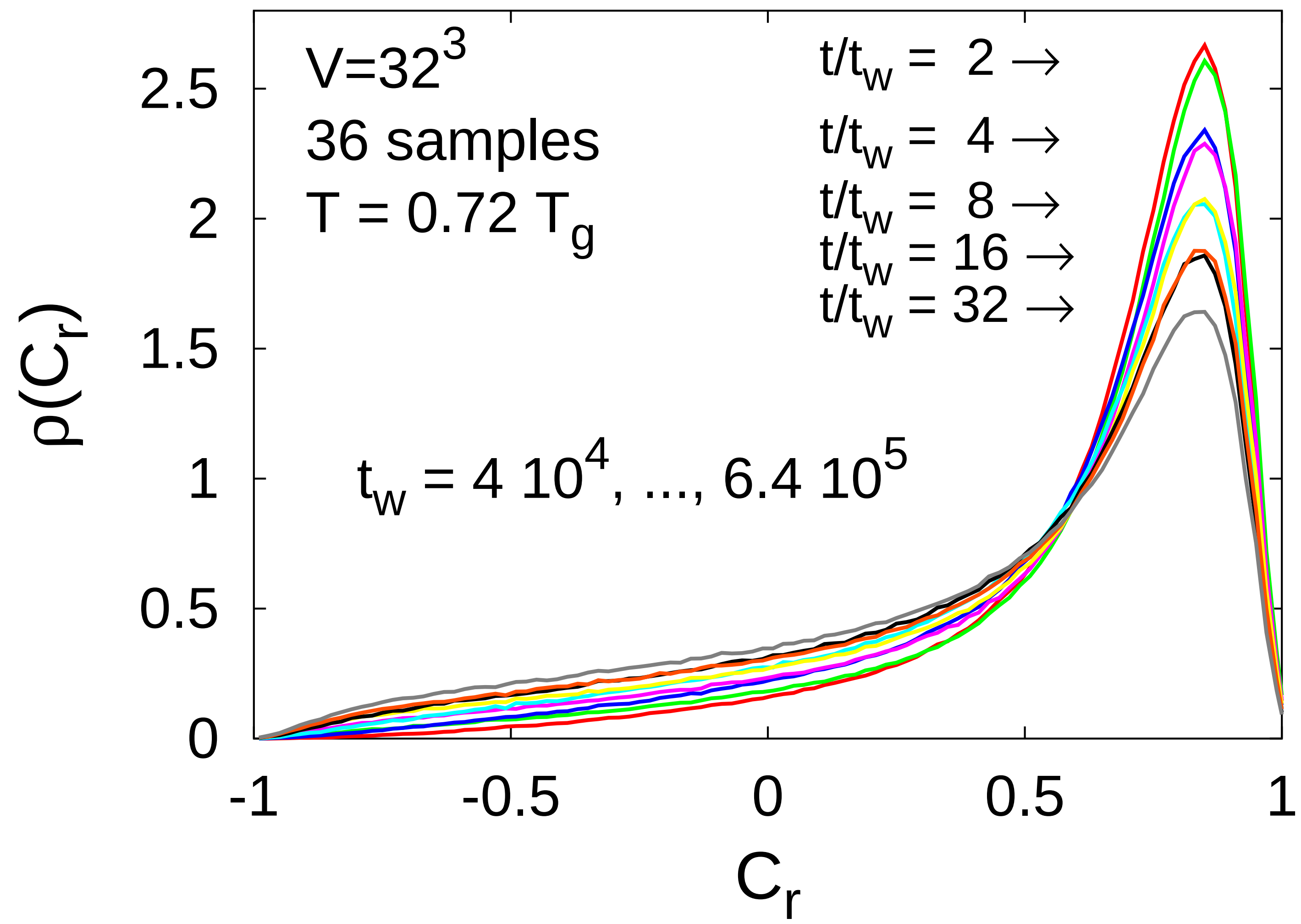


3D short-range $\pm J$ spin glass Monte Carlo

$V = 64^3$, $T = 0.72 T_g$, $t_w = 4 \times 10^4$ MCs

$t/t_w = 1.00005, 1.001, 1.06, 2, 8, 32$

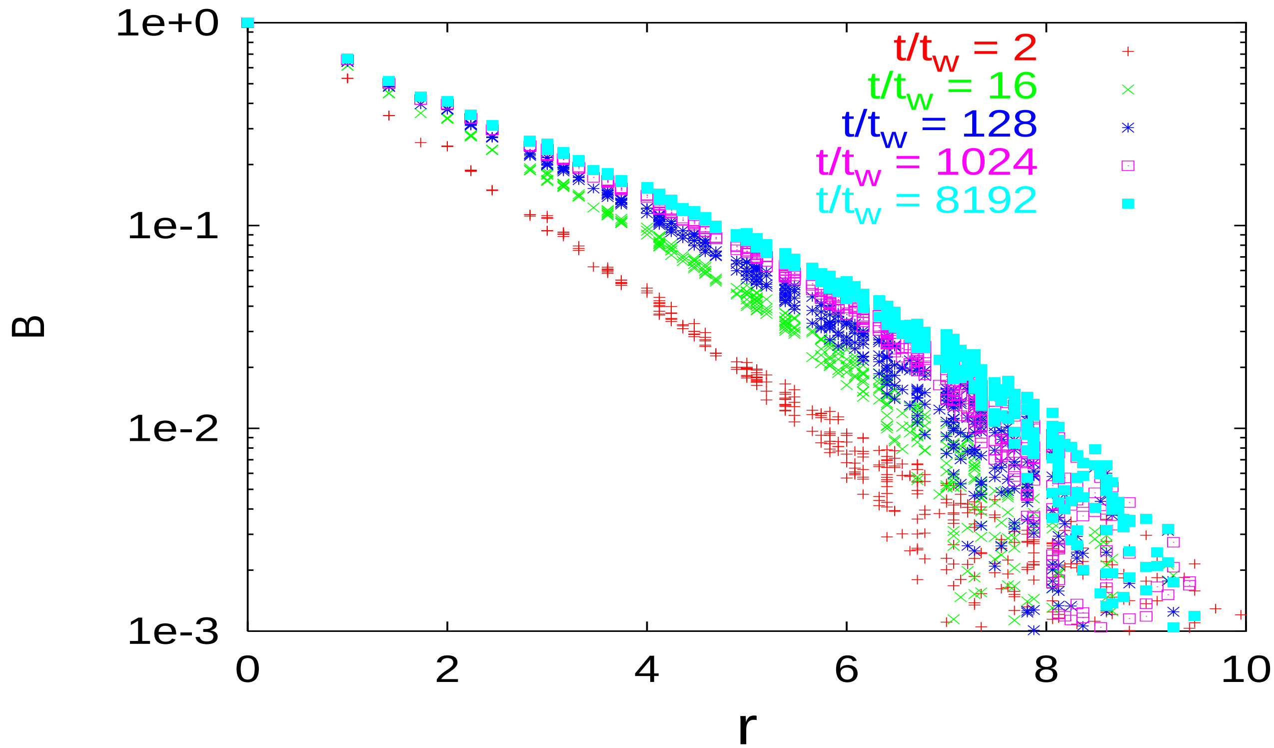
$\rho(C_{\vec{r}})$ collapses with t/t_w



Noise-noise spatial correlations: exponential decay

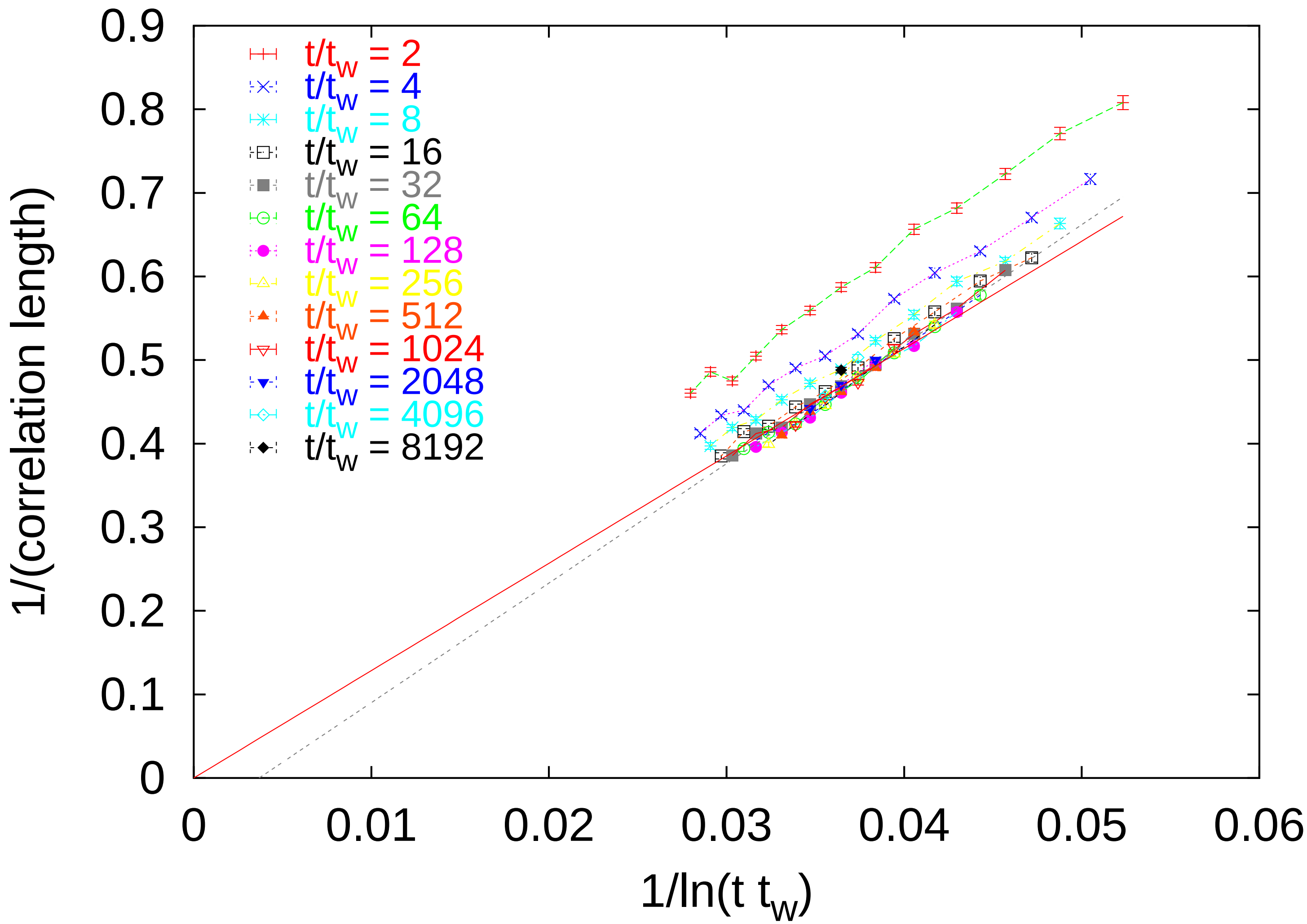
RG-irrelevant symmetry-breaking terms $\Rightarrow$ expect finite correlation length ($\to \infty$ for infinite t, t_w).

$$B(\vec{r}, t, t_w) \equiv \langle \delta C_{\vec{r}_i}(t, t_w)\ \delta C_{\vec{r}_i + \vec{r}}(t, t_w) \rangle_{\vec{r}_i}$$



$t_w = 10^4$ MCs, $V = 32^3$, $T = 0.72 T_g$, 64 disorder realizations

Correlation length $\xi(t, t_w) \to \xi(tt_w)$



$V = 32^3$, $T = 0.72T_g$, 64 disorder realizations

Outline

1. Experiments show that glasses are out of equilibrium: age-dependent effects (“Physical aging”) and “FDT violations”.

2. Symmetry under time reparametrization. Goldstone mode: space dependent ages in glassy systems.

3. Numerical evidence in models of spin glasses and structural glasses.

Structural glass simulations

- 80:20 binary Lennard-Jones mixture, 8000 particles. Thermalized at $T_i = 5.0$, time origin at instantaneous quench to $T_f = 0.4$ (below $T_g \approx 0.435$). Evolves for up to 100000 LJ units (i.e. $\sim 10^{-8}s$) after quench. β relaxation time is of the order of 1 LJ unit. Repeated for 250 to 4000 independent runs (depending on timescale).

- Divide the system in regions, and measure one point, two time quantities for each region.

  $$C_{\vec{r}}^{\text{part}}(t, t_w) \equiv \frac{1}{\mathcal{N}(V_{\vec{r}})} \sum_{\vec{r}_i(t_w) \in V_{\vec{r}}} \cos(\vec{q} \cdot [\vec{r}_i(t) - \vec{r}_i(t_w)])$$

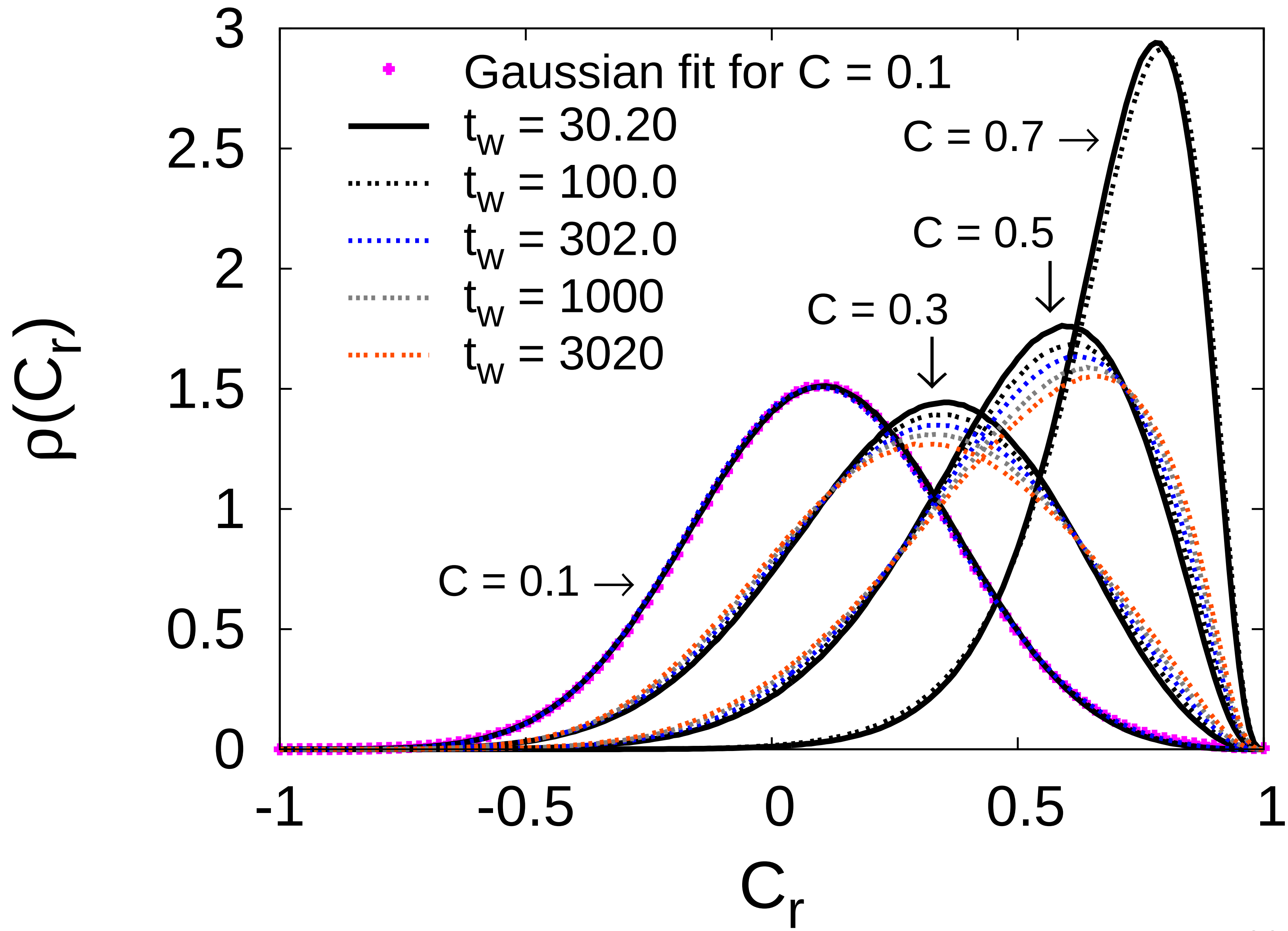
  Obtain the probability distributions $\rho(C_r)$ for the local values.

- Use the *global* intermediate scattering function

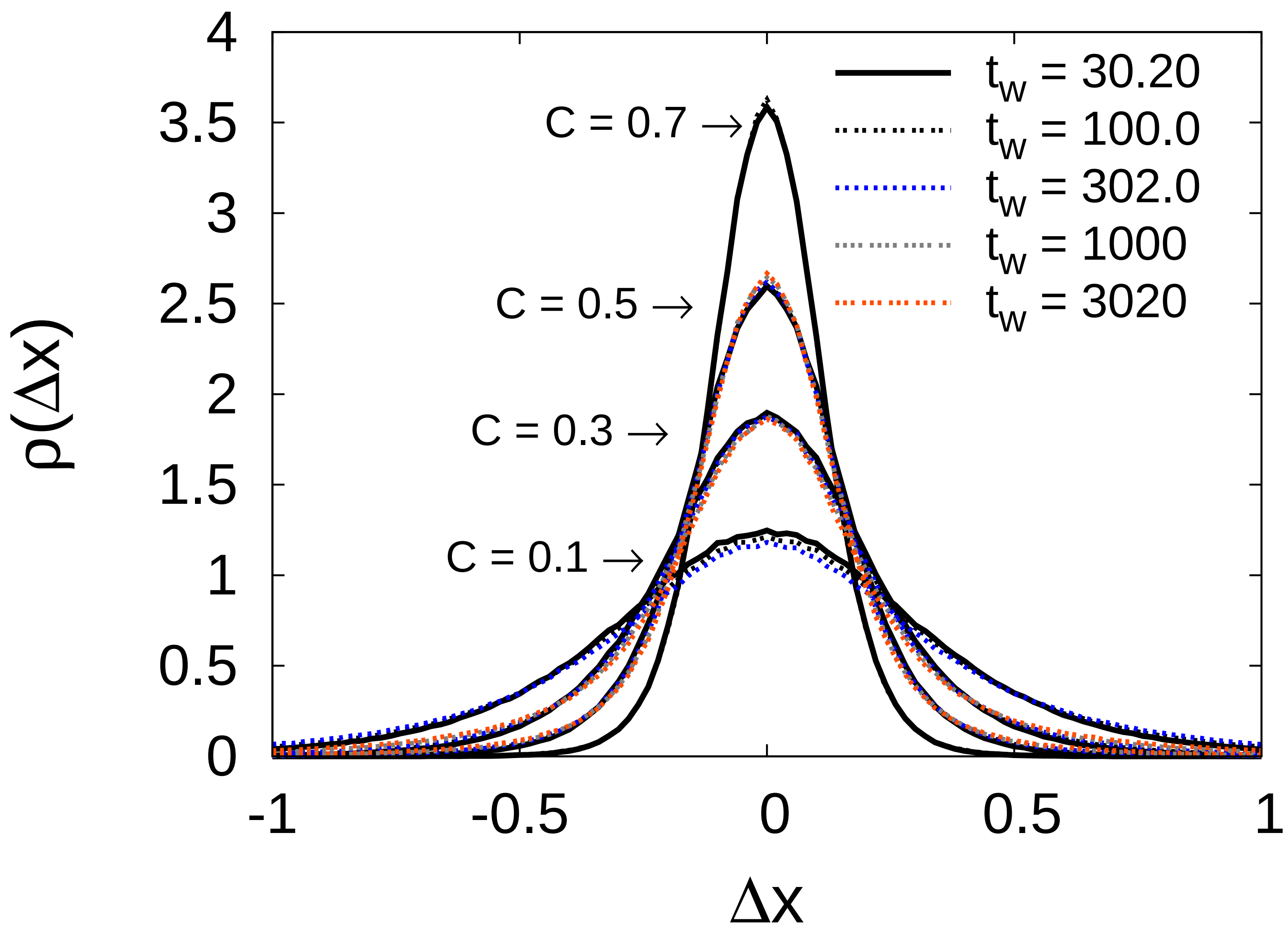
  $$C_{\text{global}}(t, t_w) \equiv \frac{1}{N} \sum_{i=1}^{N} \cos(\vec{q} \cdot [\vec{r}_i(t) - \vec{r}_i(t_w)])$$

  to quantify how correlated the system is between times t_w and t.

Approximate collapse of $\rho(C_r)$ at constant $C_{\text{global}}(t, t_w)$



Distribution of one-dimensional displacements $\rho(\Delta x)$



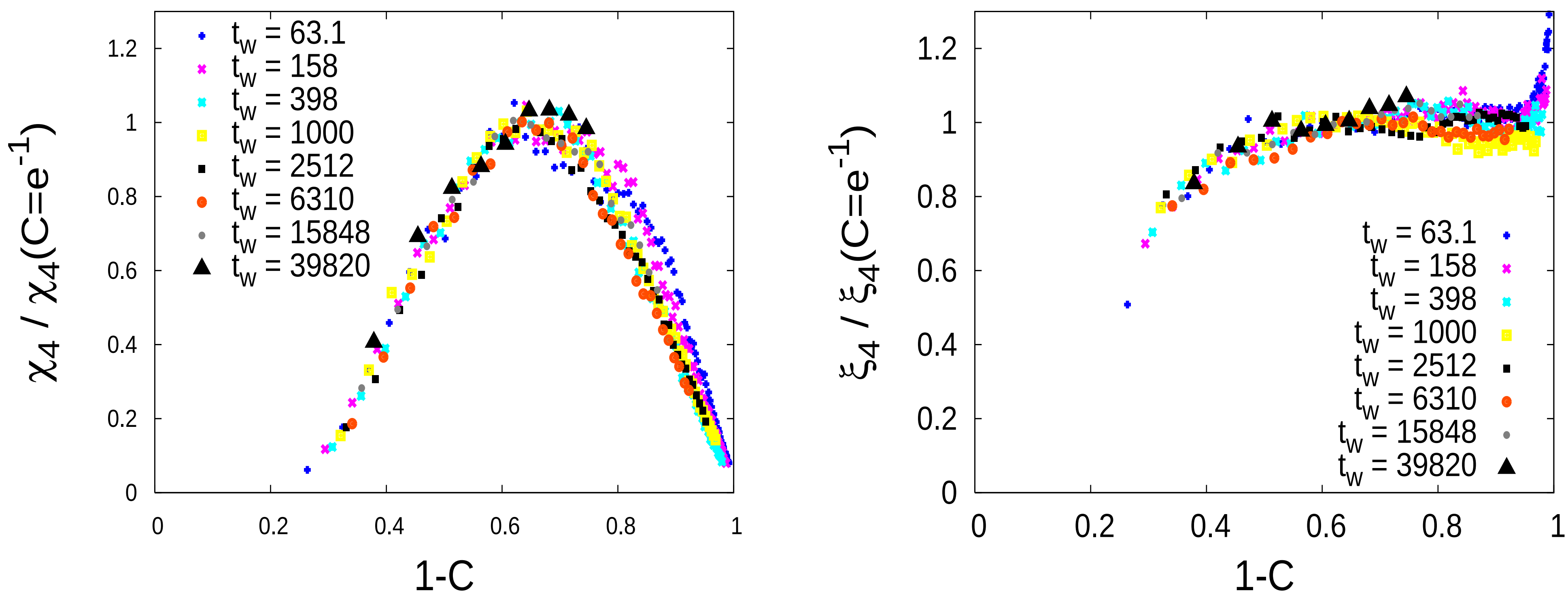
approximate collapse at constant $C_{\text{global}}(t, t_w)$.

Dynamical correlations: densities

(Lačević, Starr, Schrøder, Glotzer J. Chem. Phys **119**, 7372 (2003))

$$
\begin{aligned}
w(\mathbf{r},t,t_w) &= \text{1 if particle at } \mathbf{r} \text{ has moved} < a_{\text{vib}} \\
&= \text{0 otherwise} \\
g_4(\mathbf{r},t,t_w) &= \text{spatial correlation of } w(\mathbf{r},t,t_w) \\
\xi_4(t,t_w) &= \text{correlation length for } g_4(\mathbf{r},t,t_w) \\
\chi_4(t,t_w) &= \text{dynamic density susceptibility} \\
&\propto \int d^3r \; g_4(\mathbf{r},t,t_w)
\end{aligned}
$$

Scaled χ_4 and ξ_4 depend only on $C_{\text{global}}(t, t_w)$



Summary

- RG in **time** : In short-range spin glasses, the dynamical action is invariant under *global time reparametrizations ($t \to h(t)$)* at long times.
- Goldstone modes *(age fluctuations)* are high probability modes. These modes control the fluctuations in the aging dynamics.
- Tests in MC simulations of a 3D short-range spin glass model:
  - The distribution of $(C_{\vec{r}}, \chi_{\vec{r}})$ is concentrated on a fixed $\chi(C)$ curve.
  - $C_0(t, t_w) \approx C_0(t/t_w)$: i) the distributions of $C_{\vec{r}}$ collapse for fixed t/t_w
  - Irrelevant terms weakly break invariance at finite times: "Goldstone modes" acquire mass $m(t, t_w)$.
- Tests in MD simulation of a simple structural glass model:
  - Probability distributions of local two-time quantities like C_r and Δx approximately collapse at fixed $C_{\text{global}}(t, t_w)$.
  - Scaling of 4-point density correlation $\chi_4(t, t_w) \approx \chi_4{}^0(t_w)\phi(C(t, t_w))$, and correlation length $\xi_4(t, t_w) \approx \xi_4{}^0(t_w)\varphi(C(t, t_w))$.