On the Brownian glass

A density field-theory[1] and **an Eulerian spin limit**[2]

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[1] A. Velenich, C. Chamon (BU), LFC & D. Kreimer (BU & IHES)

arXiv :0802.3212 ; J. Phys. A (in press).

[2] C. Chamon (BU), LFC, G. Fabricius, J.L. Iguain (Argentina) & E. Weeks (Emory)

arXiv :0802.3297 ; submitted to PNAS.

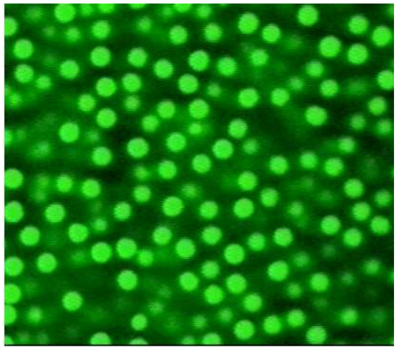
Rutgers, May 2008.

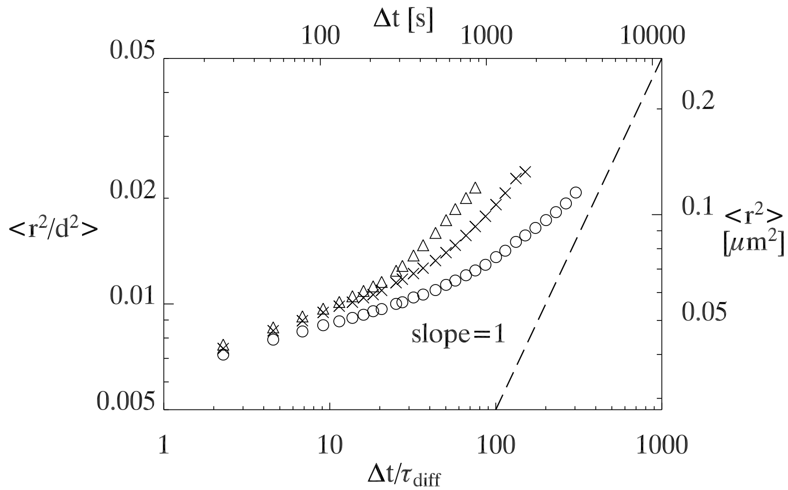
Colloidal suspensions

Micron-sized plastic beads suspended in a liquid

Observed by confocal microscopy

ϕ is the packing fraction





$Nr^2 \equiv \sum_i [\vec{x}_i(t) - \vec{x}_i(t_w)]^2$

$\Delta t \equiv t - t_w$

Slowing down with increasing ϕ in SCL

or with t_w at fixed ϕ in glass

- A dilute suspension flows like a liquid,
- It gets ‘pasty’ (super-cooled liquid) at $\phi \approx 56\%$
- At $\phi \approx 58\%$ it turns into an out of equilibrium glass.

E. R. Weeks

Interacting Brownian particles

Overdamped Langevin dynamics

$$\gamma \frac{d\vec{x}_i}{dt} = - \sum_{j(<i)} \vec{\nabla}_i V(|\vec{x}_i - \vec{x}_j|) + \vec{\xi}_i \ ,$$

$i = 1, \dots, N$ particles. $a = 1, \dots, d$ dimensions. L box linear size.

$\rho_0 = N/L^d$ mean density. $\lambda_0 = \rho_0^{-1/d}$ mean interparticle distance.

V is a **pair potential**.

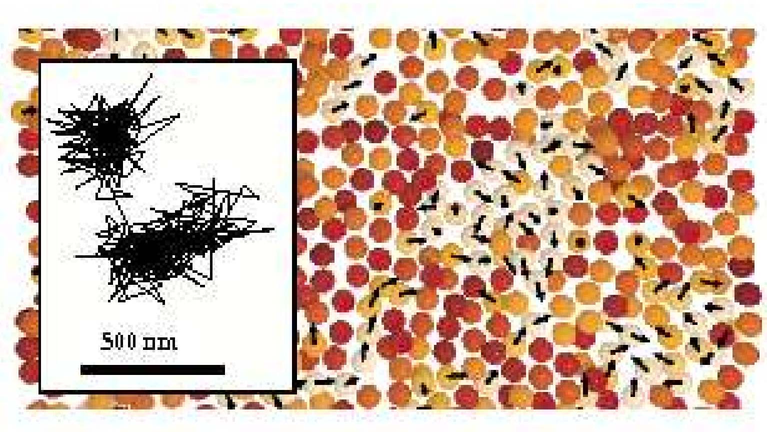
$\vec{\xi}_i$ is the **thermal Gaussian white noise** on the i-the particle :

$$\langle \, \xi_i^a(t) \, \rangle = 0 \ , \qquad \langle \, \xi_i^a(t) \xi_j^b(t') \, \rangle = 2\gamma k_B T \, \delta_{ij} \, \delta^{ab} \delta(t-t') \qquad \forall a, b \ .$$

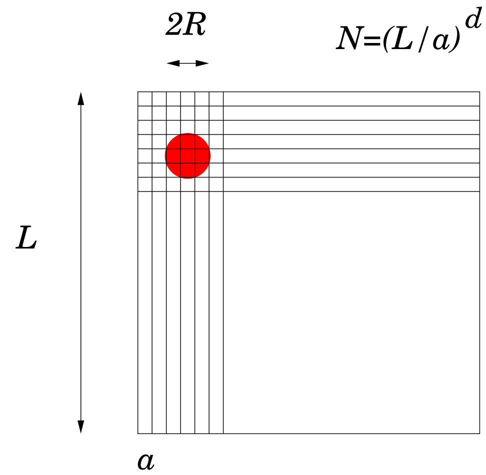
with T the temperature and $\gamma = k_B = 1$ henceforth.

One follows the individual trajectories

Eulerian analysis



Weeks & Weitz ’02



Chamon et al ’08

- Particles are *indistinguishable* ; fixed lattice reference frame.
- An Ising spin $s_i = \pm 1$ is assigned to an occupied (empty) pixel.
- $\sum_{i=1}^{N} s_i = 0$ is ensured by rescaling the particle radii, $R \to R_{eff}$.
- In the exp. $N \approx 10^3$ in $60 \times 60 \times 12 \mu m^3$,

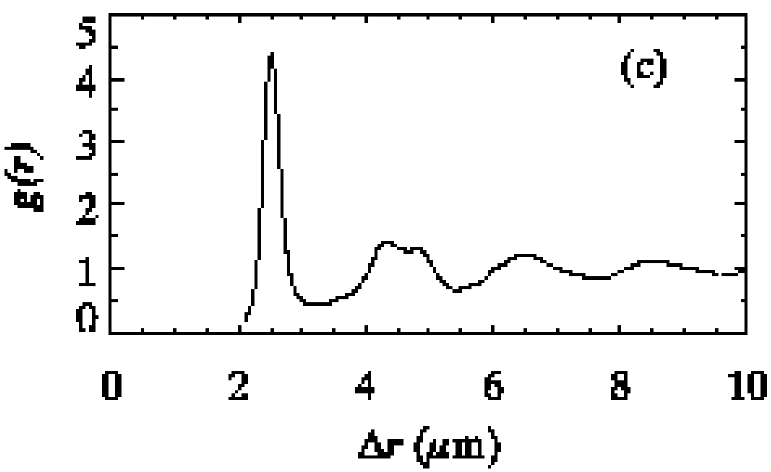
  $R = 1.18 \mu m, \; R_{eff} \approx 1.17 \mu m$.
- In the analysis $a = 0.236 \mu m$ ($\approx$ mean displacement $r \approx 0.2 \mu m$).
- There is no large-distance coarse-graining ; $\boxed{a \ll R_{eff}}$.

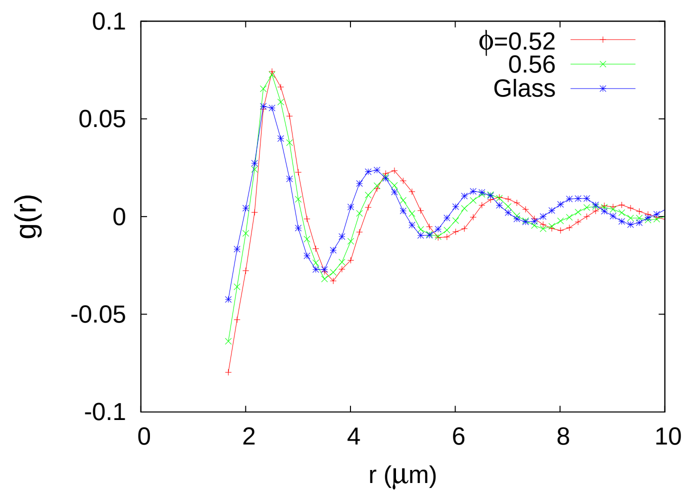
Colloidal suspensions

Pair correlation $g(r,t)$: cfr. standard definition

$\frac{1}{N}\sum_{i=1}^{N}\delta(\vec{r}-\vec{r}_i(t))$

$\frac{1}{N}\sum_{i,j;|\vec{x}_i-\vec{x}_j|=r} s_i(t)s_j(t)$





From particle trajectories

Weeks, Crocker & Weitz '06

From spins

Chamon et al '08

The same peak structure ; very weak dependence on ϕ

Colloidal suspensions

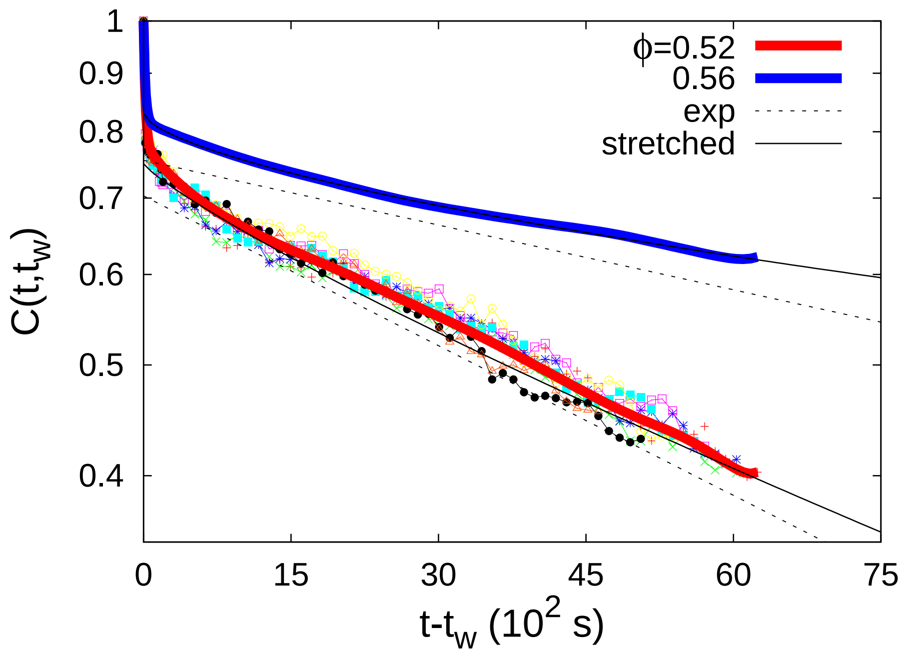
In the liquid and super-cooled liquid

low density regime

the two-time correlation

$$C(t, t_w) = \frac{1}{N} \sum_{i=1}^{N} s_i(t) s_i(t_w)$$

is stationary



Super-cooled liquid $\approx$

stretched exponential

Liquid $\approx$ exponential

Time-reversal symmetry and FDT

An overdamped Langevin process with additive white noise

The Martin-Siggia-Rose-Jenssen-de Dominicis action (in $d = 1$)

$$S = \int_t \{i\hat{x}_i[d_t x_i + d_{x_i} V(|x_i - x_j|)] + T(i\hat{x}_i)^2\}$$

is invariant under the **linear transformation** :

$t \to \tau = -t$, $\quad x_i(t) \to x_i(\tau)$, $\quad d_t x_i(t) \to -d_\tau x_i(\tau)$, and

$i\hat{x}_i(t) \to i\hat{x}_i(\tau) + \frac{1}{T} d_\tau x_i(\tau)$.

It implies that the averaged dynamics are **stationary** and

$$\langle\, i\hat{x}_j(t_w) x_i(t)\,\rangle_S = \langle\, i\hat{x}_j(t) x_i(t_w)\,\rangle_S + \frac{1}{T}\partial_{t_w}\langle\, x_i(t) x_j(t_w)\,\rangle_S$$

Identifying the linear response to a field that couples linearly to x_i, $V \to V - \sum_k h_k x_k$, one finds the **fluctuation-dissipation theorem (FDT)**

$$R_{ij}(t, t_w) \equiv \left.\frac{\delta\langle\, x_i(t)\,\rangle}{\delta h_j(t_w)}\right|_{h=0} = -\frac{1}{T}\frac{dC_{ij}(t,t_w)}{d(t-t_w)} \quad \text{for} \quad t \geq t_w$$

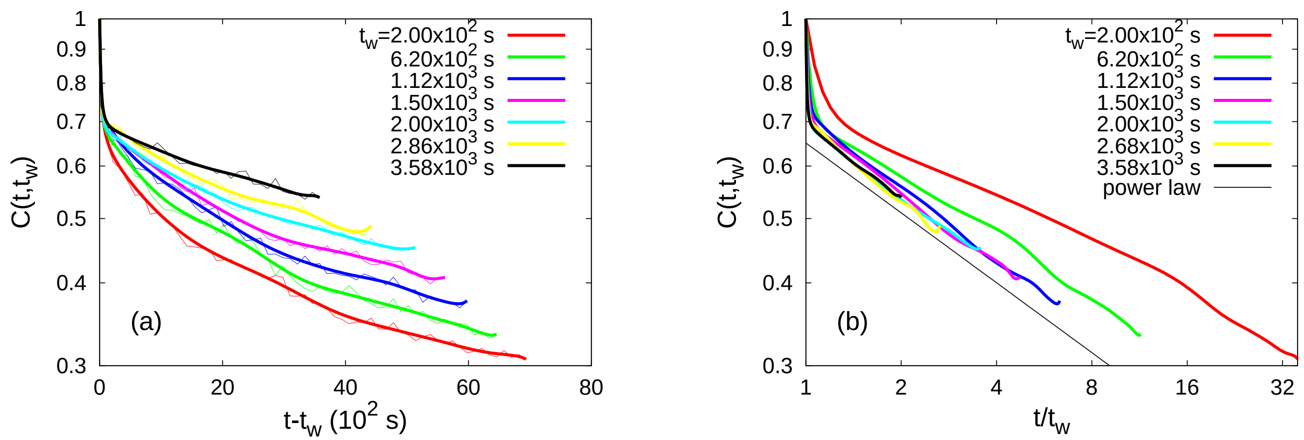
Theory : constraint

- The theory of a free relaxing liquid cannot violate the time-reveral symmetry of its MSRJD generating functional explicitly.

  Any self-consistent approximation should **preserve this symmetry**.

- During glassy relaxation time-reversal symmetry and the FDT are **sponta-neously broken** (but not explicitly !)

The two-time correlation $C(t,t_w) = \frac{1}{N}\sum_{i=1}^{N} s_i(t)s_i(t_w)$ **ages**



Density evolution

Using Itô calculus **D. S. Dean '96** showed that the local density field

$$\rho(\vec{x},t) \equiv \sum_{i=1}^{N} \delta(\vec{x}-\vec{x}_i(t)) \ ,$$

satisfies the 'Langevin' equation

$$\frac{\partial \rho(\vec{x},t)}{\partial t} = \vec{\nabla}\left(\rho(\vec{x},t)\vec{\nabla}\frac{\delta F[\rho]}{\delta \rho(\vec{x},t)}\right) + \vec{\nabla}\left(\vec{\eta}(\vec{x},t)\sqrt{\rho(\vec{x},t)}\right) \ ,$$

with the **'free-energy'**

$$F[\rho] \equiv \frac{1}{2}\int_{\vec{x}\vec{y}} \rho(\vec{x},t)V(|\vec{x}-\vec{y}|)\rho(\vec{y},t) + T\int_{\vec{x}} \rho(\vec{x},t)\ln\rho(\vec{x},t)$$

and **multiplicative Gaussian noise** $\vec{\eta}$ with $\langle\, \eta^a(\vec{x},t)\,\rangle = 0$ and

$$\langle\, \eta^a(\vec{x},t)\eta^b(\vec{y},t')\,\rangle = 2T\ \delta^{ab}\delta(\vec{x}-\vec{y})\delta(t-t') \ .$$

Generating functional

$\mathcal{Z}[J] = \int \mathcal{D}\rho \mathcal{D}i\hat{\phi}\; e^{S[\rho, i\hat{\phi}]}$ with the MSRJD action

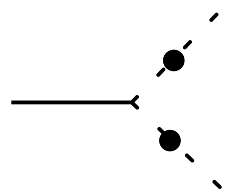
$$S[\rho, i\hat{\phi}] = \int_{\vec{x}t} \left\{ i\hat{\phi}(\partial_t - T\nabla^2)\rho + T\rho(\vec{\nabla} i\hat{\phi})^2 - i\hat{\phi}\vec{\nabla}[\rho\vec{\nabla}(\rho \star \mathbf{V})] \right\}$$

and $\rho \star \mathbf{V} \equiv \int_y \rho(\vec{y}, t)\mathbf{V}(|\vec{x} - \vec{y}|)$. No constraint on the integration measure. Note that $\langle\, \rho \,\rangle = \rho_0$.

$i\hat{\phi}$ ρ

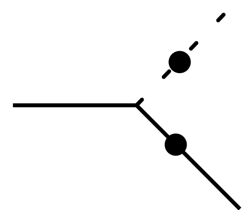
$\theta(t)e^{-Tk^2 t}$

Propagator



$-2T\vec{k}_1\vec{k}_2$

Noise vertex



$-\vec{k}_1\vec{k}_2\mathbf{V}(k_2)$

Potential vertex

The points represent the k factors.

A good starting point to develop approximations but

a very peculiar field-theory.

Non-linear time-reversal sym.

A natural perturbing field, h, couples linearly to the density and modifies the free-energy as $\mathcal{F} \to \mathcal{F} - \int_{\vec{x}} \rho(\vec{x},t) h(\vec{x},t)$. The linear response is

$$R_{\vec{x}\vec{y}}(t,t_w) = \left. \frac{\delta \langle\, \rho(\vec{x},t)\, \rangle}{\delta h(\vec{y},t_w)} \right|_{h=0} = - \left\langle\, \rho(\vec{x},t) \vec{\nabla} \left(\rho(\vec{y},t_w) \vec{\nabla} i\hat{\phi}(\vec{y},t_w) \right) \right\rangle_S$$

The time-reversal symmetry of the MSRJD action for Dean's equation is the non-linear transformation

$$t \to \tau = -t \qquad i\hat{\phi}(\vec{x},t) \to i\hat{\phi}(\vec{x},\tau) + f(\vec{x},\tau) \qquad \vec{\nabla}(\rho \vec{\nabla} f) = \frac{1}{T} \frac{\partial \rho(\vec{x},\tau)}{\partial \tau}$$

that leads to **stationarity** and the **FDT** between correlation of the density fluctuations and linear response :

$$R_{\vec{x}\vec{y}}(t,t_w) = -\frac{1}{T} \frac{dC_{\vec{x}\vec{y}}(t,t_w)}{d(t-t_w)} \qquad\qquad t \geq t_w$$

(The Jacobian equals one.)

Mode coupling approximation

Goal : derive Mode-coupling theory eqs. from Dean's field theory

- Perturbation theory up to a given (typically second) order.

  Replace bare by dressed propagators. **Kawasaki '70**

- Linear symmetries are preserved.

  S-K Ma ; Andreanov, Biroli & Lefèvre '05

- Non-linear symmetries ? They may be linearized before proceeding.

  Chamon & LFC ; Andreanov, Biroli & Lefèvre '05

  Still, ultraviolate divergencies for Dean's field theory (in, e.g., the equation fixing the plateau in the correlation function).

What is the origin of the problem ?

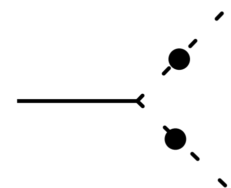
The Brownian gas : $V = 0$

$\rho = \rho_0 + \varrho$ implies $\mathcal{L} = \underbrace{i\hat{\phi}(\partial_t - T\nabla^2)\varrho + T\rho_0(\vec{\nabla} i\hat{\phi})^2} + T\varrho(\vec{\nabla} i\hat{\phi})^2$.

Propagators

$\rho_0 e^{-Tk^2|t|}$ $\qquad$ $\theta(t)e^{-Tk^2 t}$ $\qquad$ $\theta(-t)e^{Tk^2 t}$

The theory is non-Gaussian, **noise vertex** : $\quad -2T\vec{k}_1\vec{k}_2$



The **non-linear time-reversal symmetry** is still present.

How does one recover the Poissonian statistics,

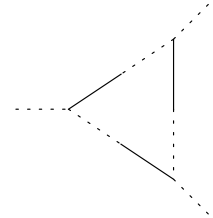
$$\langle \varrho(\vec{x}_1, t) \ldots \varrho(\vec{x}_n, t)\rangle_c = \lambda_0 \, \delta(\vec{x}_1 - \vec{x}_n) \ldots \delta(\vec{x}_{n-1} - \vec{x}_n) \; ,$$

with $\lambda_0 = \rho_0^{-d}$ the mean interparticle distance ?

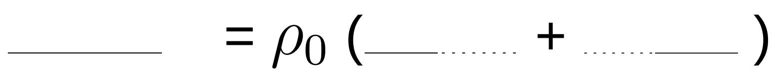
Very easy from the individual Langevin equations but from the field-theory ?

The Brownian gas : $V = 0$

Simplification : **loop diagrams vanish** due to **causality**



Just **tree diagrams**.



Propagator decomposition $\rho_0 e^{-Tk^2|t|} = \rho_0[\theta(t)e^{-Tk^2 t} + \theta(-t)e^{Tk^2 t}]$

Diagram decomposition, magic combinatorics and **graph cancellation** leads to the **expected Poissonian statistics** for all n.

The generic **FDT** between n-point correlations and their associated responses can be explicitly checked. Importantly enough, the non-linear symmetry and the $\vec{k}$ structure of the vertex lead to cancellations between diagrams of **different rank**.

The noise vertex encodes the discrete particle nature.

No problem with the $V = 0$ field theory.

Some questions & ideas

How to deal with the $V \neq 0$ case ?

- Can one control the perturbation theory without introducing extra fields to linearize the symmetry ?

- Is there another self-consistent approximation leading to the k-structure in MCT and no divergencies ?

- Naive power-counting : non-renormalizability... Can Hopf algebras help ?

A. Velenich, C. Chamon, LFC, D. Kreimer (in progress)

- Alternative approach : can one obtain the k-dependence in the **mode-coupling** theory from an 'equivalent disorder model' ? More precisely, which is the **random manifold** to be used ?

A. Sicilia & LFC (in progress)

Conclusions

– We have proposed a simple way to **collect and analyze** experimental data from confocal microscopy measurements in particle systems and numerical data from molecular dynamics simulations.

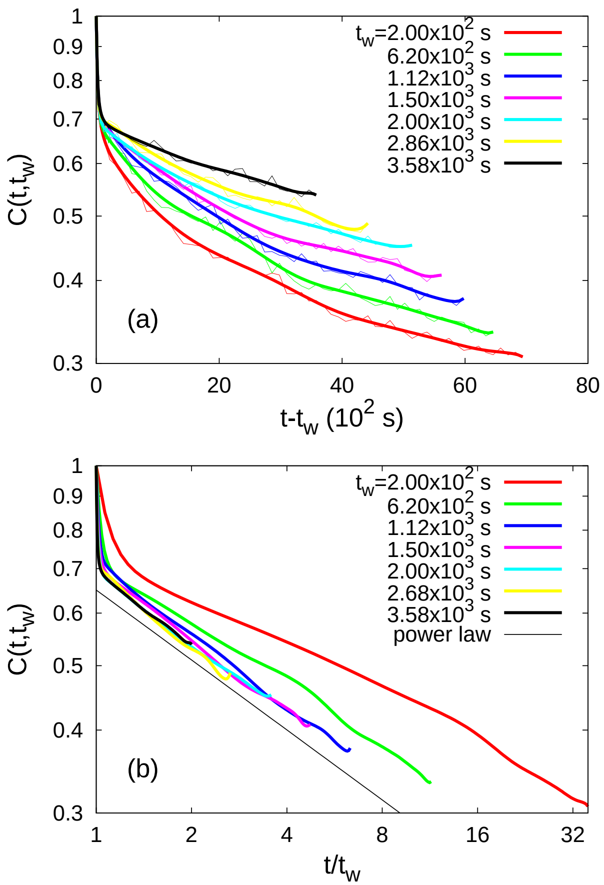
  It might be useful to make the relation to **spin coarsening and glassy models** more quantitative as well as to ‘derive’ **kinetically constrained spin models**.

– A step forward in the understanding of a **density field-theory** for colloidal suspensions : the discrete particle nature is encoded in the noise vertex. Some ideas to go on in this direction.

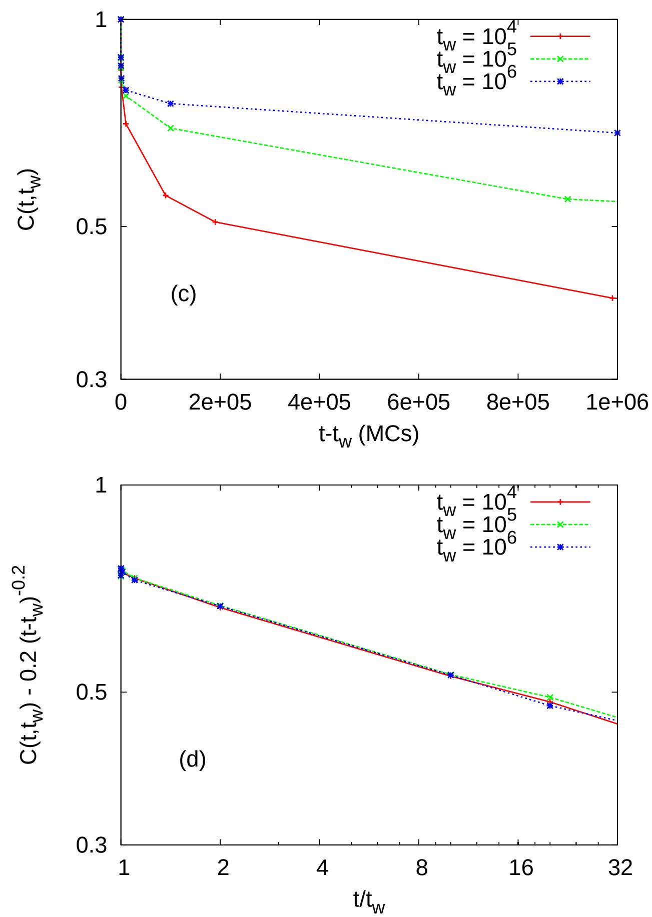
  Can one argue for asymptotic time-reparametrization invariance in this theory ?

Global correlation

$$C(t, t_w) = \frac{1}{N} \sum_i^N s_i(t) s_i(t_w)$$



Colloidal suspension

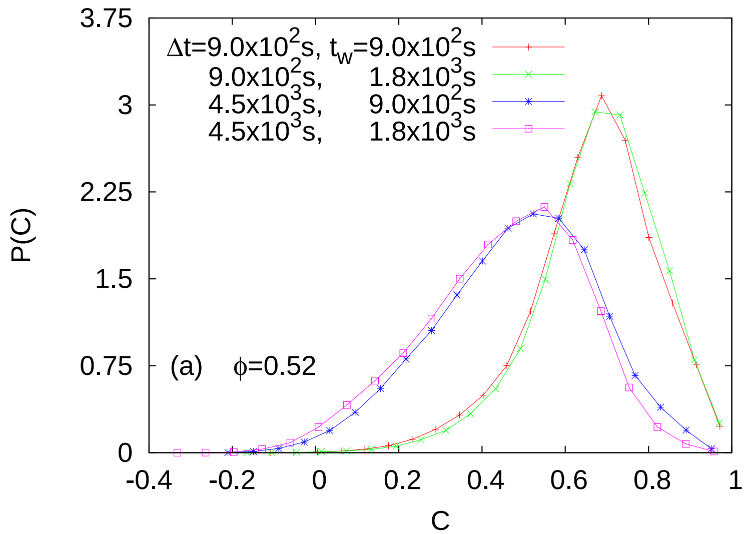


Spin-glass

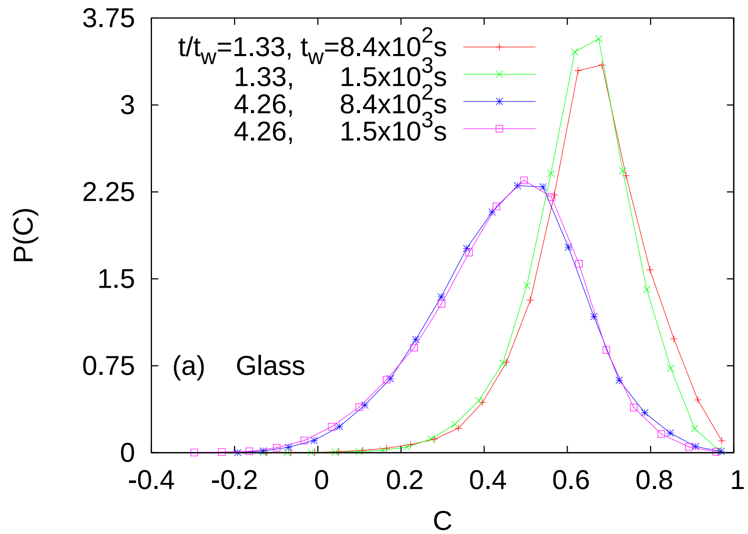
Colloidal suspensions

Pdf of local two-time function $C_r(t,t_w) = \frac{1}{n}\sum_{i\in V_r}^{n} s_i(t)s_i(t_w)$

cfr. Spin models



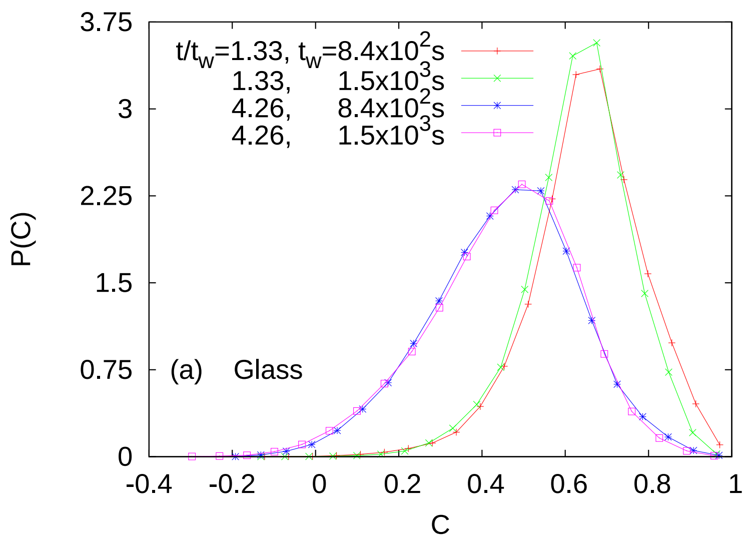
Liquid



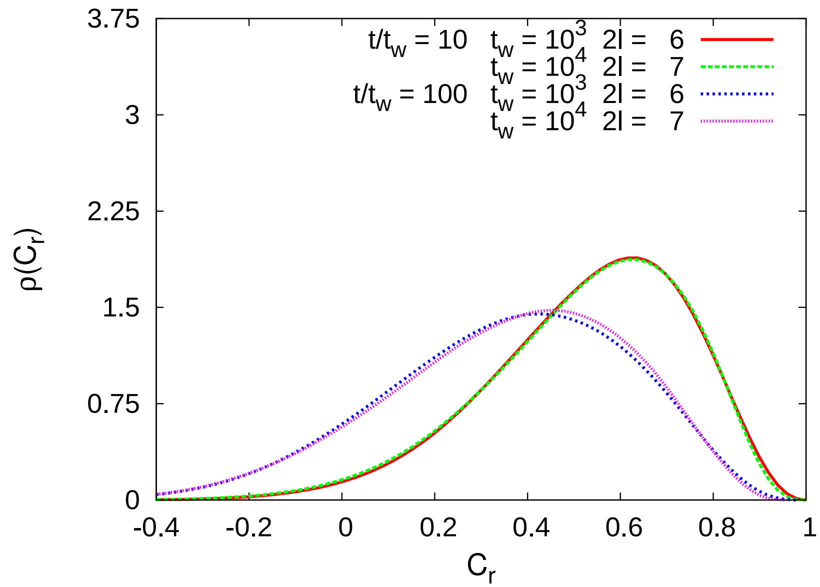
Glass

Fluctuations

Pdf of local two-time function $C_r(t, t_w) = \frac{1}{n}\sum_{i\in V_r}^{n} s_i(t)s_i(t_w)$



Colloidal suspension



Spin-glass