Effective temperatures in active matter

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Phys. Rev. E **77**, 051111 (2008), Soft Matter **7**, 3726, *ibid* **7**, 10193 (2011)

Work in collaboration with Davide Loi and Stefano Mossa.

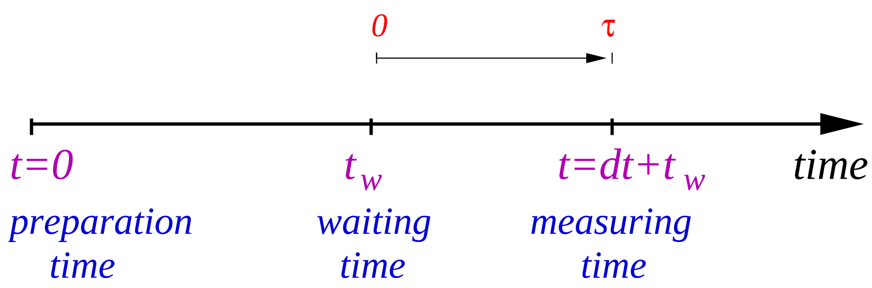
Lyon France May 2012.

In and out of equilibrium

Take a mechanical point of view and call $\{\vec{r}_i\}(t)$ the variables

e.g. particles' coordinates $\{\vec{x}_i(t)\}$ and momenta $\{\vec{p}_i(t)\}$

Choose an initial condition $\{\vec{r}_i\}(0)$ and let the system evolve.



- For $t_w > t_{eq}$: $\{\vec{r}_i\}(t)$ reach the equilibrium pdf and thermodynamics and statistical mechanics apply. **Temperature** is a well-defined concept.

- For $t_w < t_{eq}$: the system remains out of equilibrium and thermodynamics and (Boltzmann) statistical mechanics **do not** apply.

Is there a quantity to be associated to a temperature ?

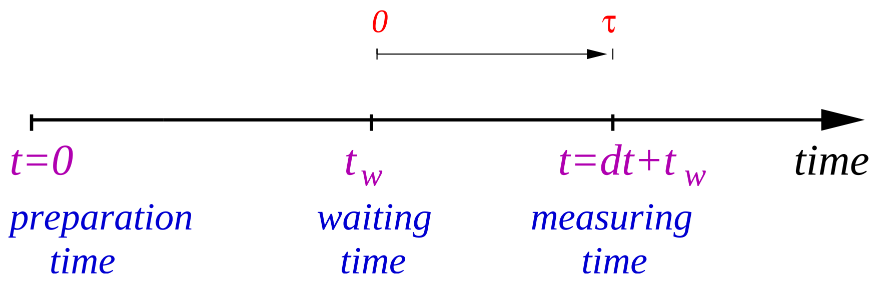
Non-potential forces

Let $\{\vec{x}_i\}(t)$ be the positions of the (possibly interacting) particles.

Apply external forces that do not derive from a potential, $\vec{f}_i \neq -\vec{\nabla}_i V(\{\vec{x}\})$:

energy injection into the system.

Let the system evolve under $\vec{f}_i$ from $\{\vec{r}_i\}(0)$.

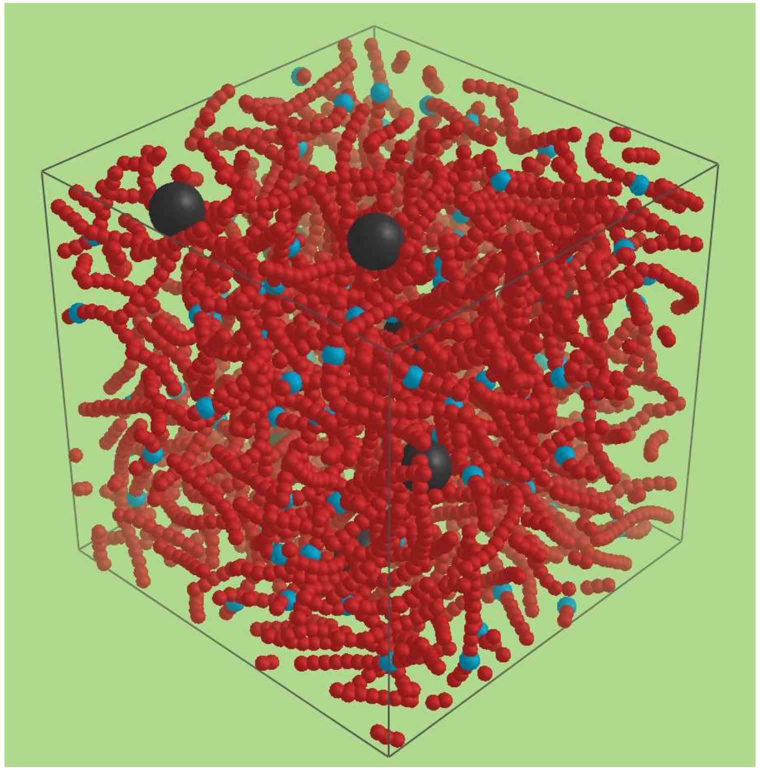


- Typically, for $t_w > t_{st}$: $\{\vec{r}_i\}(t)$ reach a non-equilibrium steady state in which thermodynamics and (Boltzmann) statistical mechanics do not obviously apply.

Is there a quantity to be associated to a temperature ?

Active matter

The polymer example



Molecular dynamics

Point-particles or linear molecules

$\vec{f}_i^d$ deterministic force

Lennard-Jones potential

$\vec{f}_i^M$ stochastic motor forces

act during τ

on $\%$ particles

$$m_i \dot{\vec{v}}_i + \gamma \vec{v}_i = \vec{f}_i^d(\{\vec{x}_j\}) + \vec{f}_i^M + \vec{\xi}_i$$

Loi, Mossa & LFC 08-11

The passive model

Forces

$$\vec{f}^{\,d}_{ai} = - \sum_{b(\neq a)}^{N_p} \sum_{j=1}^{N_m} \vec{\nabla}_{bj} V_{inter}(r_{aibj}) - \sum_{j=1}^{N_m} \vec{\nabla}_{bj} V_{intra}(r_{aibj})$$

mechanical force acting on monomer i in polymer a exerted by the other monomers in the same and different polymers.

The inter and intra polymer potentials are of **Lennard-Jones type** :

$$V_{inter}(r) = \left\{ 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \epsilon \right\} \theta(2^{1/6}\sigma - r)$$

$$V_{intra}(r) = \begin{cases} k(r - r_0)^2 & \text{nn} \\ \left\{ 4\epsilon \left[\left(\frac{S}{r}\right)^{12} - \left(\frac{S}{r}\right)^{6} \right] + \epsilon \right\} \theta(2^{1/6}\sigma - r) & \text{next nn} \end{cases}$$

Unit of energy, $2k_BT$, of length 0.4 nm, of force 20 pN at ambient temperature.

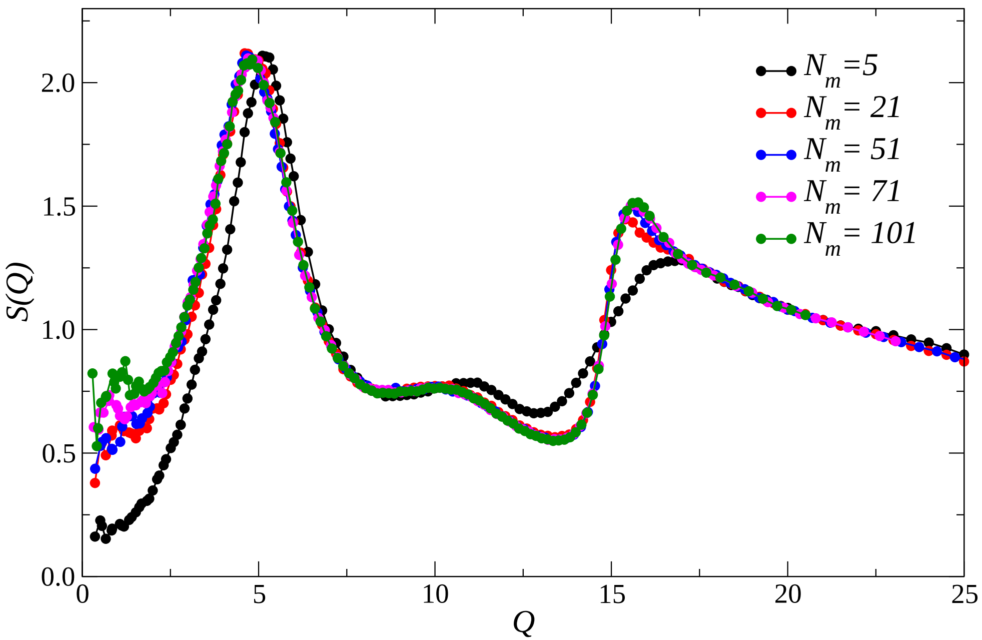
Interacting polymers

Structure of the passive model

Parameters such that lines are semi-flexible $\boxed{S = 2.5\, r_0}$ in liquid phase

Miura et al. Phys. Rev. E 63, 061807 (2001).

For $N_p = 250$ and $\rho = 1$, N_m–independent structure factor for $N_m \gtrsim 21$.



1st peak

$q_0^{-1} \;\simeq\;$ nn distance

(typically $a \neq b$)

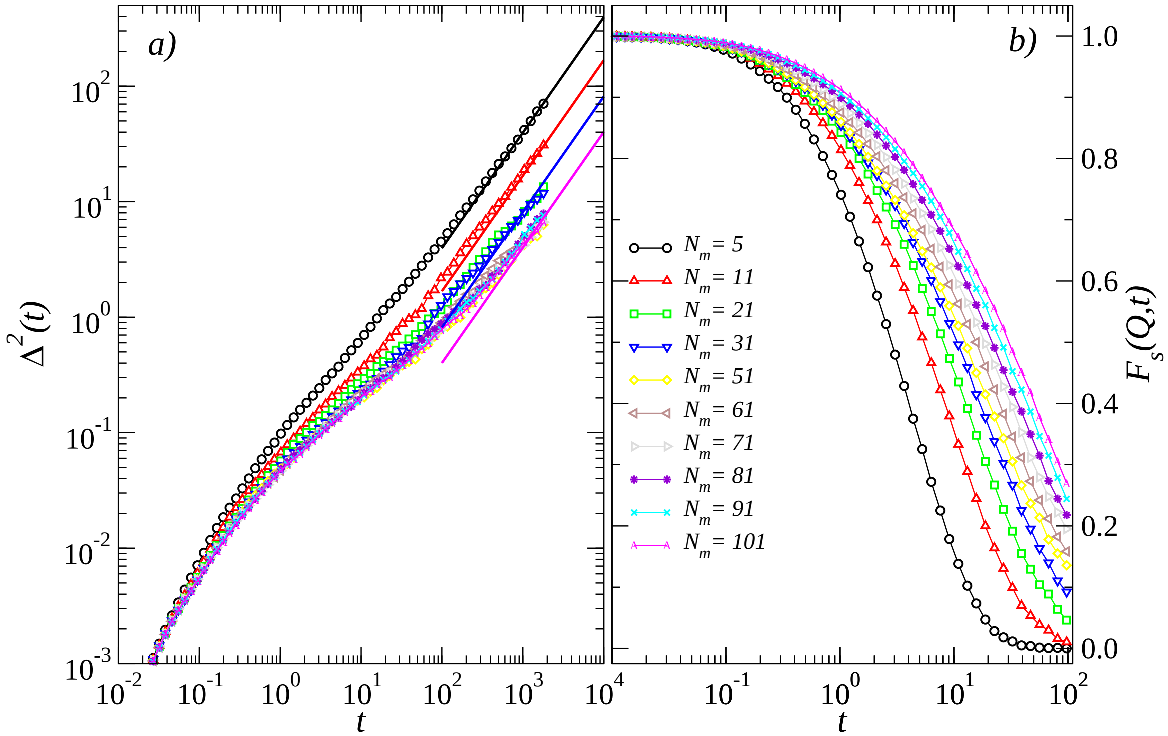
2nd peak

$q_1^{-1} \;\simeq\;$ equil. bond r_0

Analysis of radius of gyration : non-Gaussian chains.

Interacting polymers

Dynamics of the passive model



$D \simeq N_m^{-1}$

$\tau_\alpha \simeq N_m^{3/4}$

for

$N_m \lesssim 50$

We'll use

$N_m = 21$

$$\Delta^2(t) = \frac{1}{N_p N_m} \sum_{a=1}^{N_p} \sum_{i=1}^{N_m} |\vec{r}_{ai}(t+t_0) - \vec{r}_{ai}(t_0)|^2$$ Mean-square displacement

$$F_s(Q,t) = \frac{1}{N_p N_m} \sum_{a=1}^{N_p} \sum_{i=1}^{N_m} e^{i\vec{Q}[\vec{r}_{ai}(t+t_0) - \vec{r}_{ai}(t_0)]}$$ Incoherent scattering

Active matter

Adamant motor activity

Requirements :

– Homogeneously distributed in the sample.

– Motor acts at the center of the polymers (OK on short time-scales).

– Linear response regime.

Intensity given by a fraction of the conservative mechanical force of the passive system

$$|\vec{f}_{ai}^{M}| = f \, \frac{1}{N_p N_m} \sum_{a=1}^{N_p} \sum_{i=1}^{N_m} |\vec{f}_{ai}^{d}| = f \, \overline{F} \qquad \overline{F} \simeq 163.5$$

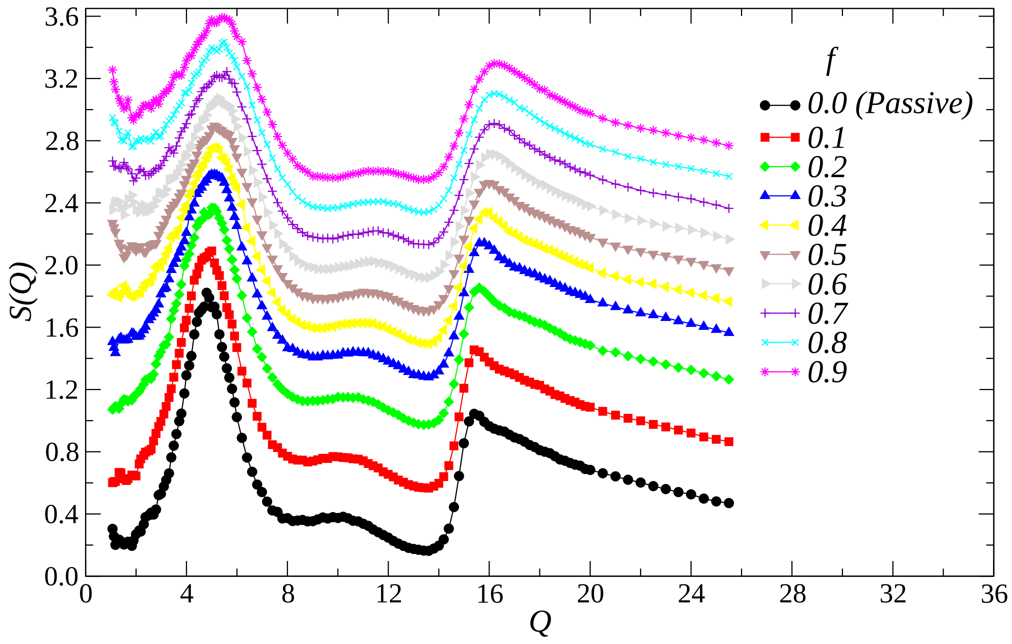
– Time series of randomly applied kicks on % polymers.

– Activation time scale $\tau = 500$ MDs : constant $\vec{f}_{ai}^{M}$ over this period.

The motor action is independent of the structural rearrangements induced

Active matter

Structure properties



1st peak $\longrightarrow$ right :

nn dist. decreases, *i.e.*

crowding.

Width increases &

height decreases, *i.e.*

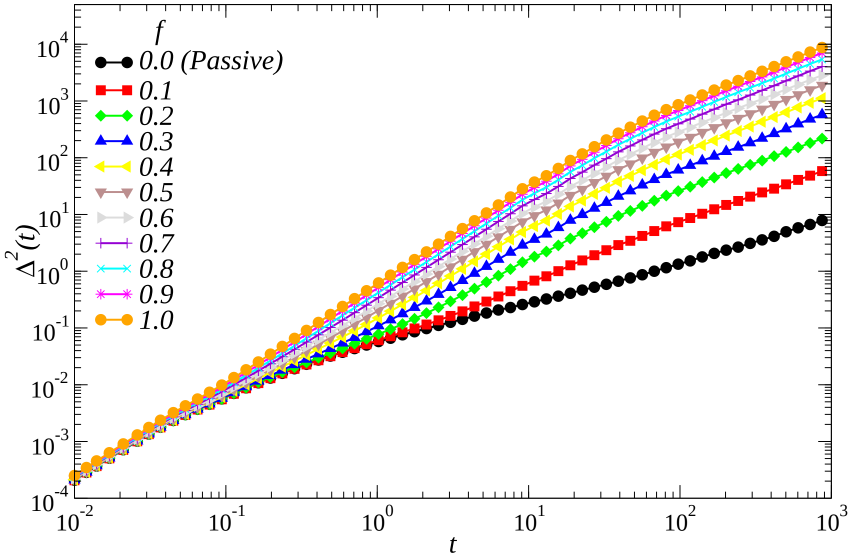
disorder.

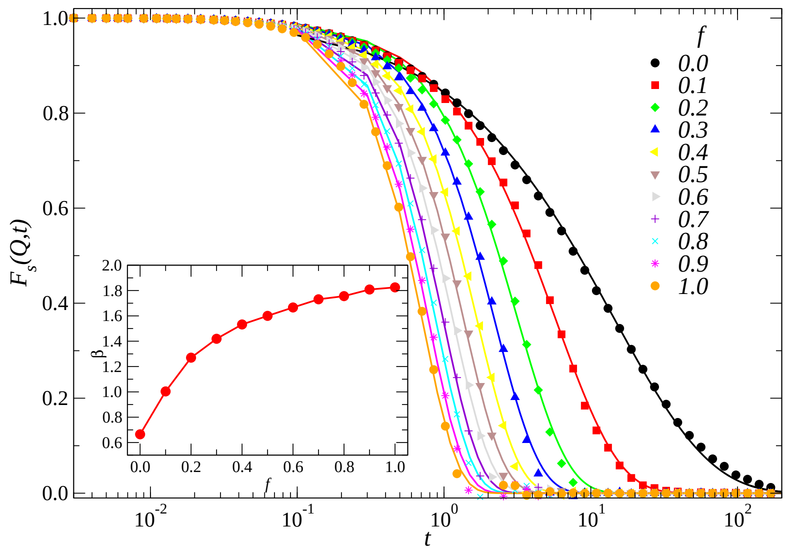
Averaged radius of gyration decreases with increasing f : chain folding.

Complex dependence of its pdf with f.

Active matter

Dynamics





$$D/D_0 \simeq 1+1423\, f^{2.29}$$

$$(\tau/\tau_0)^{-1} \simeq 1 + 19\, f$$

Could the exponent be actually 2 and $D/D_0 \simeq 1 + c\, \mathrm{Pe}^2$ as in

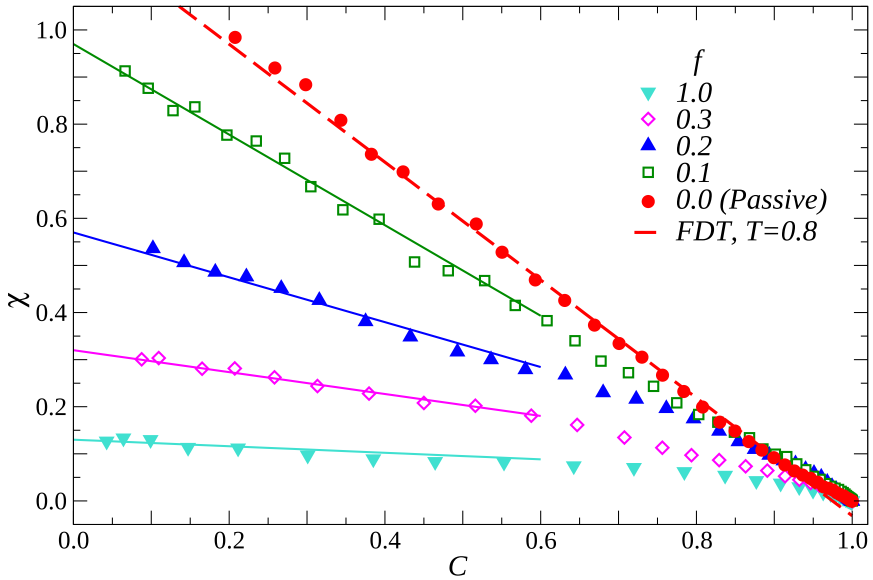
J. Palacci, C. Cottin-Bizonne, C. Ybert, and L. Bocquet, PRL 105, 088304 (2010)

with $\mathrm{Pe} = f$ here ?

(Recall $\mathrm{Pe} = vR/D_0$.)

Active matter

Integrated linear response against correlation function



$$C(t-t_w) \propto \sum \langle e^{i\vec{q}_0[\vec{x}(t)-\vec{x}(t_w)]}\rangle$$

$$\chi(t-t_w) \propto \sum \int_{t_w}^{t} dt' \left.\frac{\delta\langle e^{i\vec{q}_0\vec{x}(t)}\rangle}{\delta h(t')}\right|_{h=0}$$

$$H \to H - 2h \sum \epsilon \cos(\vec{q}_0\vec{x})$$

Sums over all monomers

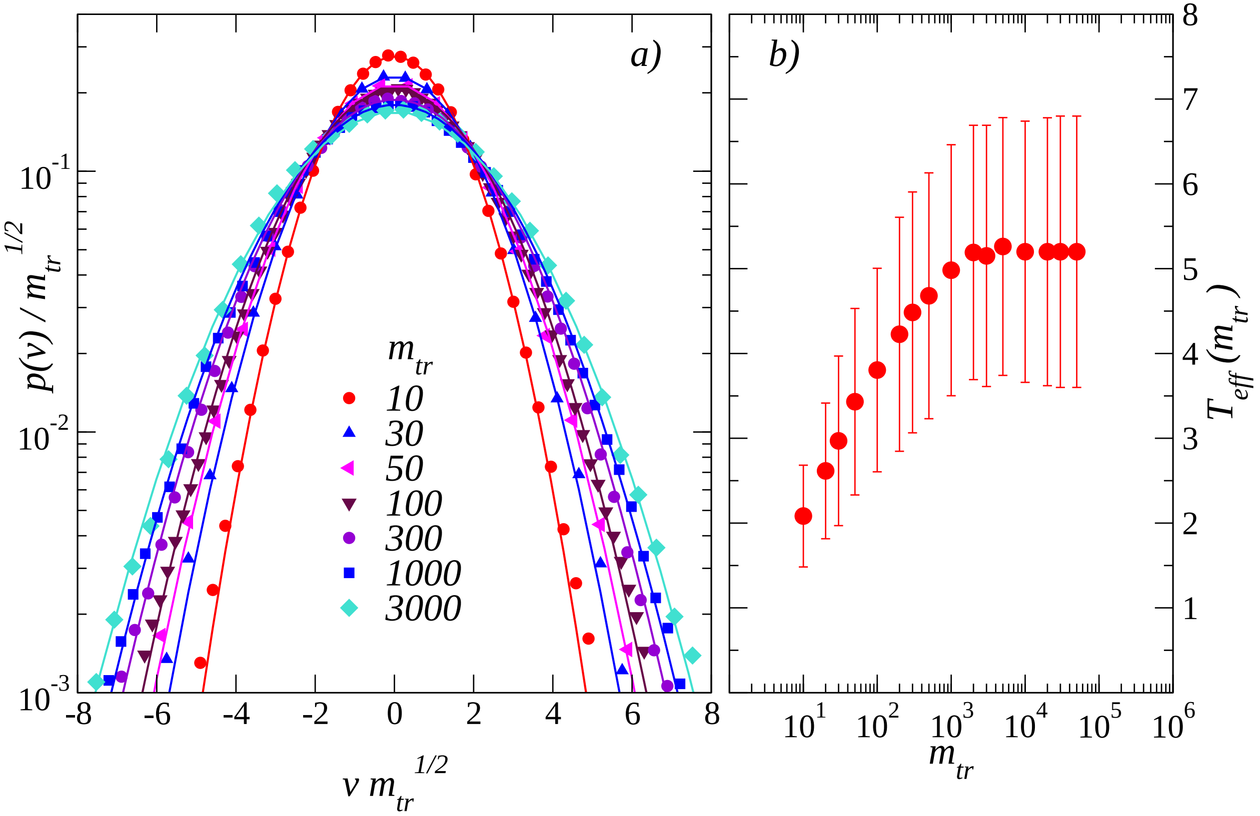
$$\chi(t-t_w) = \frac{1}{T_{\rm eff}(t-t_w)}\left[C(0) - C(t-t_w)\right]$$

In equilibrium $T_{\rm eff}(t-t_w) = T$. Here, $T_{\rm eff}(f) =$ ct $> T$, for small C.

Active matter

Tracers' velocities

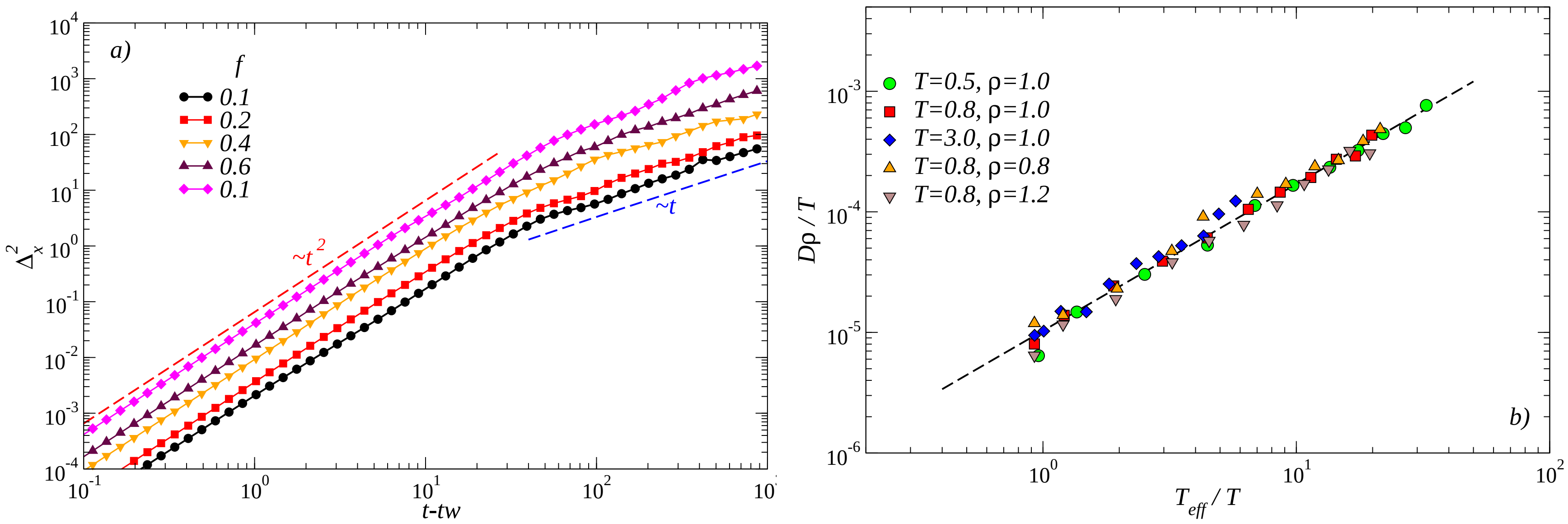
Spherical particles with mass m_{tr} that interact with the active matter.



Maxwell pdf of tracers' velocities v at an effective temperature $T_{\rm eff}(m_{tr})$.

Active matter

Tracers' diffusion

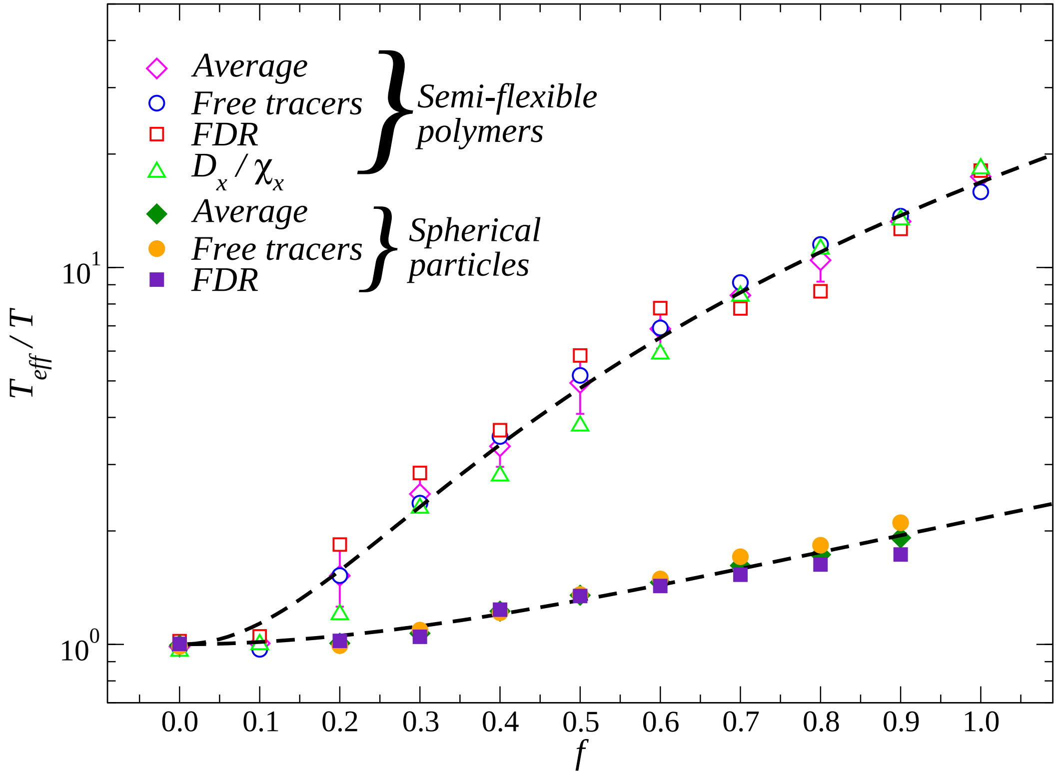


$$\Delta_x^2(t, t_w) = \langle [\vec{x}(t) - \vec{x}(t_w)]^2 \rangle \simeq 2D_x |t - t_w|$$

Brownian motion : $D_x \propto T$ **in active matter** $D_x \propto T_{\text{eff}}$

Active matter

Effective temperature dependence on activation



$$\boxed{T_{\text{eff}}/T \simeq 1 + c\, f^2} \qquad \stackrel{?}{=} 1 + c\,\text{Pe}^2$$

$c \simeq 15.41$ for filaments and $c \simeq 1.18$ for particles.

Active matter

Work in progress

- Totally randomly acting (adamant) motors yield $T_{\rm eff} > T$
- Would susceptible motors yield $T_{\rm eff} < T$?

  This happens when heating a zero-temperature ground state in, e.g., the $2d$ XY model or an elastic line in random media

  Berthier, Holdsworth, Sellitto 01 & Iguain, Bustingorry, Kolton, LFC 09

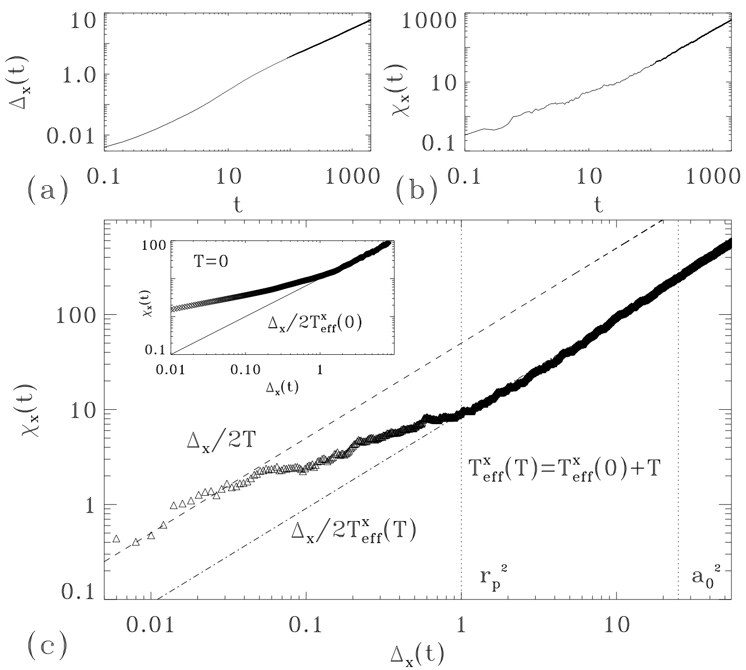
- Could this "dynamic cooling" stabilize a crystalline phase ?

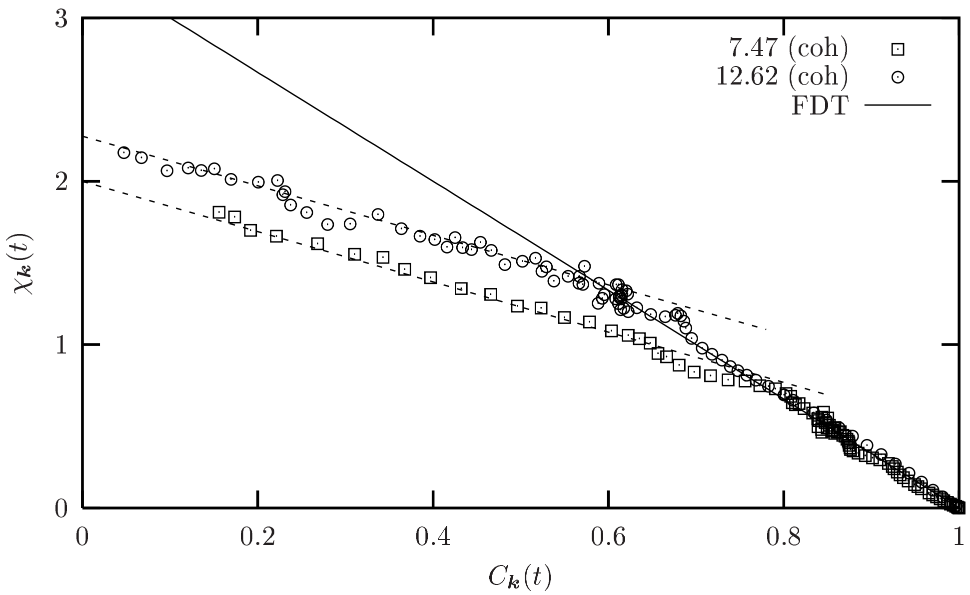
  Shen, Wang & Wolynes 04-11

Work in progress with **Mossa (Grenoble), Gonnella, Laghezza & Lamura (Bari), Arenzon & Hernandez (Porto Alegre).**

FDT in driven systems

Simulations





Driven Bragg glass

Lennard-Jones binary mixture

A. Kolton, D. Domínguez et al 03

L. Berthier & J-L Barrat 00