Active dumbbells

Leticia F. Cugliandolo

Université Pierre et Marie Curie
Sorbonne Universités

leticia@lpthe.jussieu.fr
www.lpthe.jussieu.fr/˜leticia

Work in collaboration with

D. Loi & S. Mossa (Grenoble, France, 2007-2009) and

G. Gonnella, P. Di Gregorio, G.-L. Laghezza, A. Lamura, A. Mossa & A. Suma

(Bari & Trieste, Italia, 2013-2015)

Palma de Mallorca, España, 2017

Plan

5 lectures & 2 exercise sessions

1. Introduction
2. Active Brownian dumbbells
3. Effective temperatures
4. Two-dimensional equilibrium phases
5. Two-dimensional collective behaviour of active systems

Third lecture

Plan

5 lectures & 2 exercise sessions

1. Introduction
2. Active Brownian dumbbells
3. **Effective temperatures**
4. Two-dimensional equilibrium phases
5. Two-dimensional collective behaviour of active systems

Plan

3rd Lecture

1. General discussion
2. Single active dumbbell
3. Collective active dumbbells
4. Interacting polymers with adamant motors
5. Experiments
6. Discussion

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3rd Lecture

1. **General discussion**
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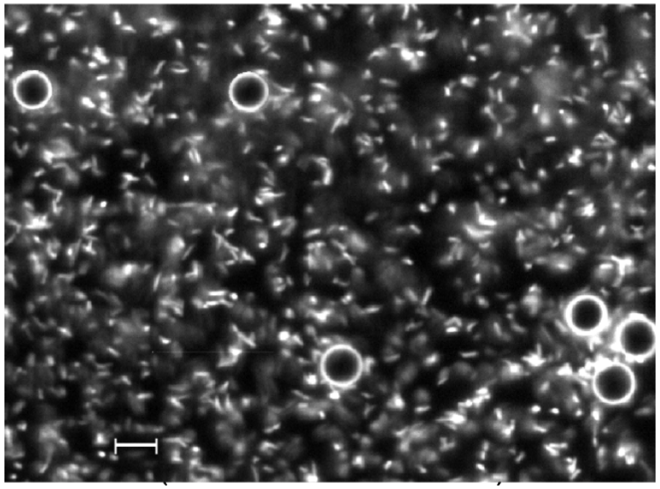
An active bath



Dynamics of an *open system*

The system : the Brownian particle

A double bath : bacteria suspension

Interaction

'Canonical setting'

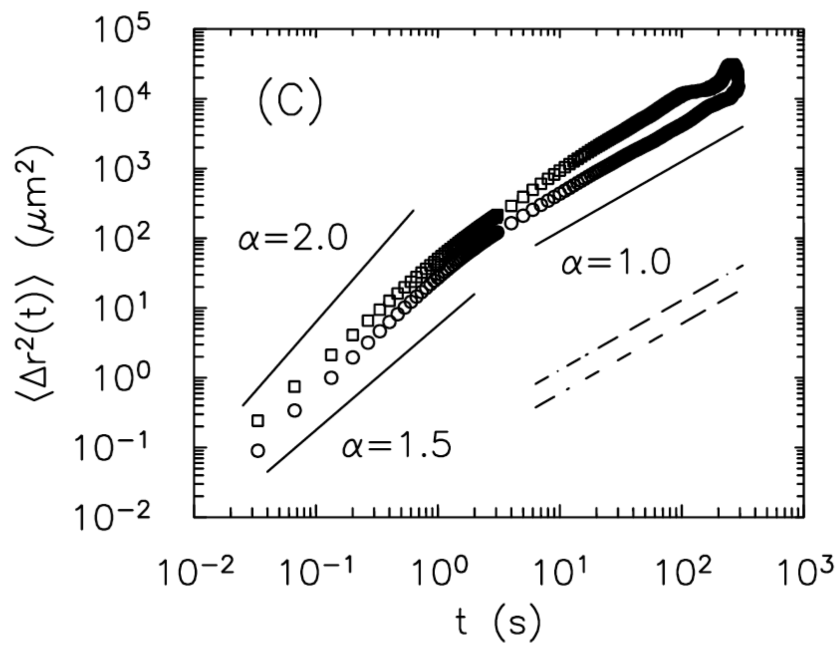
A few Brownian particles or tracers ● imbedded in an active bath

"Particle Diffusion in a Quasi-Two-Dimensional Bacterial Bath"

Wu & Libchaber, Phys. Rev. Lett. 84, 3017 (2000)

An active bath

Enhanced motility



Mean-square displacement of the Brownian particle

crossover form super-diffusion to diffusion

enhanced diffusion constant: effective temperature

$t_I = m/\gamma \simeq 10^{-5}\, s$ and the first ballistic regime is not visible.

$D_{\rm eff} \propto T_{\rm eff}$ increases with ϕ and corresponds to $T_{\rm eff} \simeq 100\, T$

"Particle Diffusion in a Quasi-Two-Dimensional Bacterial Bath"

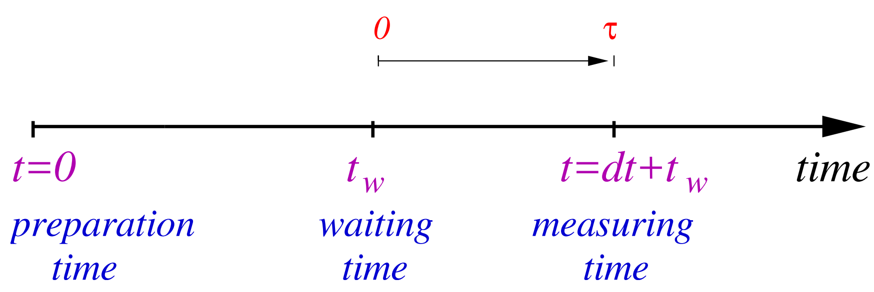
Wu & Libchaber, Phys. Rev. Lett. 84, 3017 (2000)

In and out of equilibrium

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

e.g. particles' coordinates $\{\boldsymbol{r}_i(t)\}$ and velocities $\{\boldsymbol{v}_i(t)\}$

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



- For $t_w > t_{eq}$: $\{\zeta_i\}(t)$ 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 ?

In and out of equilibrium

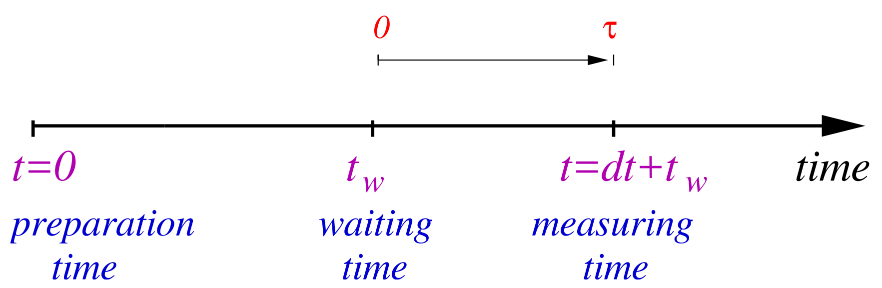
Non-potential forces

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

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

energy injection into the system.

Let the system evolve under $\boldsymbol{f}_i$ from $\{\zeta_i\}(0)$



- Typically, for $t_w > t_{\rm st}$: $\{\zeta_i\}(t)$ 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 ?

Some basic properties

requested

Control of heat-flows : ΔQ follows ΔT.

Partial equilibration – transitivity :

$T_A = T_B, T_B = T_C \Rightarrow T_A = T_C$.

Measurable :

thermometers for systems in

good thermal contact (ΔQ)

Whatever we identify with a temperature should have these properties

Kinetic temperature

First temptation

Associate a kinetic temperature $T_{\rm kin}$ to the kinetic energy via

$$k_B T_{\rm kin}(t_0) = m[\langle v_a^2(t_0)\rangle]$$

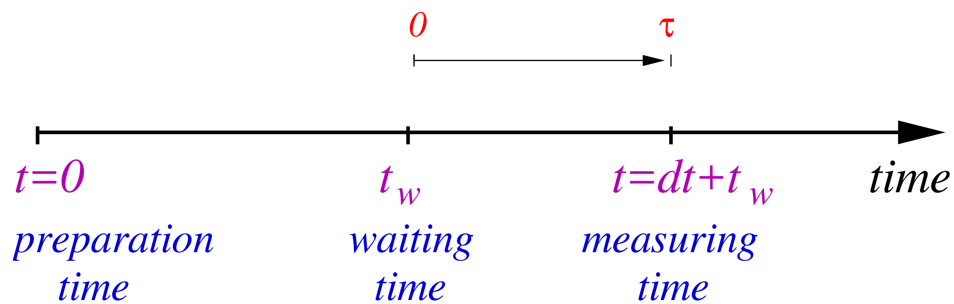
equipartition. This is an instantaneous measurement. But, we know that

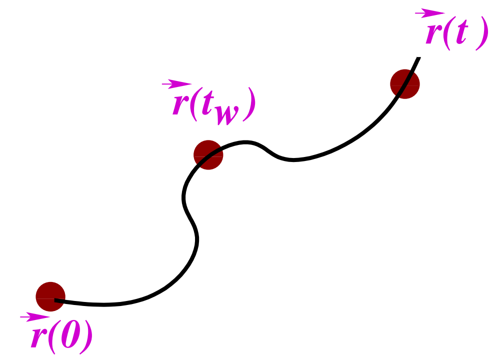
- the behaviour of the system depends on the time-delay at which we measure (recall e.g. the various regimes of the c.o.m. displacement $\Delta_{\rm cm}(t+t_0,t_0)$,
- in glasses the kinetic temperature is not a good measurement of out of equilibrium behaviour,

we need to consider time-delayed measurements

Two-time observables

Correlations





t_w not necessarily longer than $t_{\rm eq}$.

Note change in names given to times (notation)

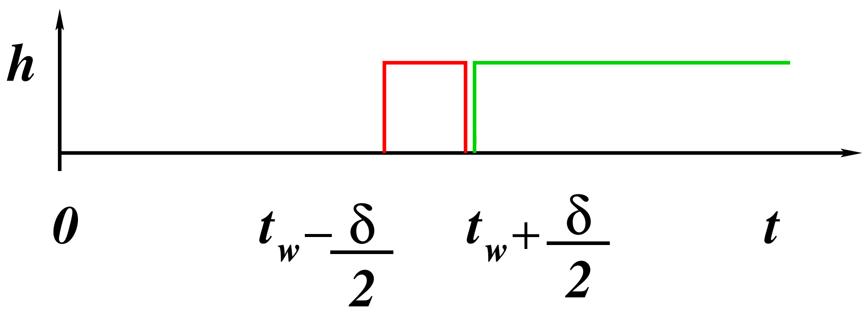
The two-time correlation between $A[\boldsymbol{\zeta}(t)]$ and $B[\boldsymbol{\zeta}(t_w)]$ is

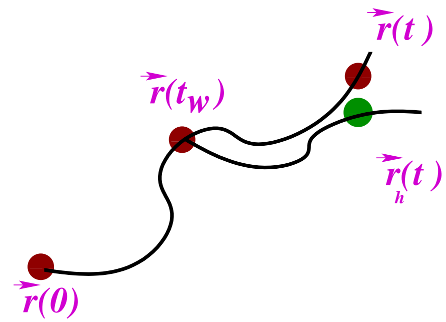
$$C_{AB}(t,t_w) \equiv \langle\, A[\boldsymbol{\zeta}(t)] B[\boldsymbol{\zeta}(t_w)]\,\rangle$$

average over realizations of the dynamics (initial conditions, random numbers in a MC simulation, thermal noise in Langevin dynamics, etc.)

Two-time observables

Linear response





The perturbation couples linearly to the observable $B[\boldsymbol{\zeta}(t_w)]$

$$E \;\to\; E - hB[\boldsymbol{\zeta}(t_w)]$$

The linear instantaneous response of another observable $A[\boldsymbol{\zeta}(t)]$ is

$$R_{AB}(t,t_w) \equiv \left.\frac{\delta\langle A[\boldsymbol{\zeta}(t)]\rangle_h}{\delta h(t_w)}\right|_{h=0}$$

The linear integrated response is

$$\chi_{AB}(t,t_w) \equiv \int_{t_w}^{t} dt'\, R_{AB}(t,t')$$

Rue de Fossés St. Jacques et rue St. Jacques

Paris 5ème Arrondissement.

LFC

Fluctuation-dissipation

In thermal equilibrium

$$\boxed{P(\zeta, t_w) = P_{\rm eq}(\zeta)}$$

- The dynamics are stationary

$$C_{AB} \to C_{AB}(t - t_w) \text{ and } R_{AB} \to R_{AB}(t - t_w)$$

- The fluctuation-dissipation theorem between spontaneous (C_{AB}) and induced (R_{AB}) fluctuations

$$R_{AB}(t - t_w) = -\frac{1}{k_B T} \frac{\partial C_{AB}(t - t_w)}{\partial t} \, \theta(t - t_w)$$

holds and implies

$$\boxed{\chi_{AB}(t - t_w) \equiv \int_{t_w}^{t} dt' \, R_{AB}(t, t') = \frac{1}{k_B T}[C_{AB}(0) - C_{AB}(t - t_w)]}$$

Fluctuation-dissipation

Linear relation between χ and C

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Fluctuation-dissipation

Linear relation between χ and Δ

$$P(\zeta, t_w) = P_{\rm eq}(\zeta)$$

- The dynamics are stationary

$$\Delta_{AB}(t, t_w) = \langle [A(t) - B(t_w)]^2 \rangle = 2[C_{AA}(0) + C_{BB}(0) - C_{AB}(t - t_w)]$$

$$\to \Delta_{AB}(t - t_w)$$

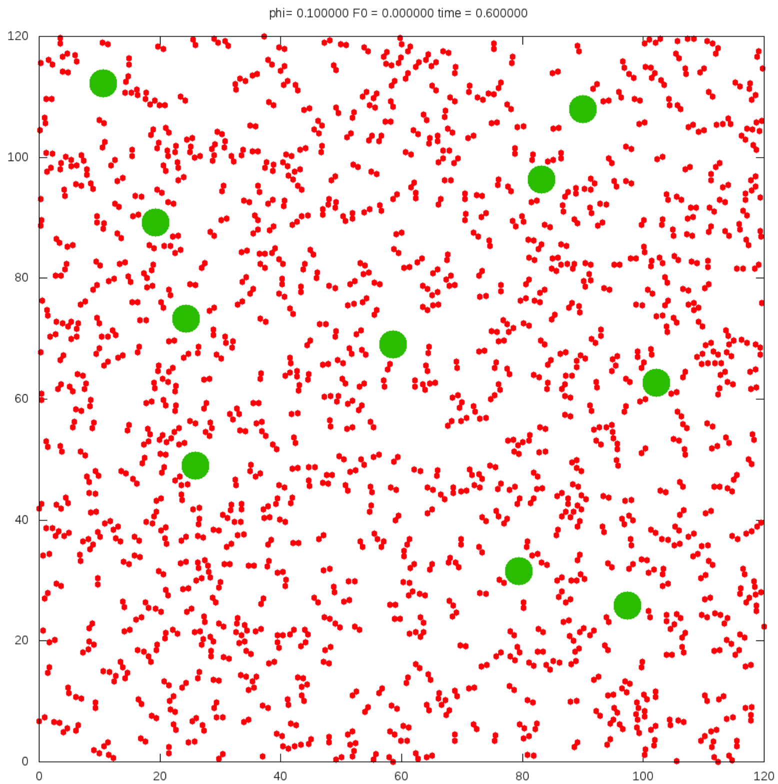
- The fluctuation-dissipation theorem between spontaneous (Δ_{AB}) and induced (R_{AB}) fluctuations

$$R_{AB}(t - t_w) = \frac{1}{2k_B T} \frac{\partial \Delta_{AB}(t - t_w)}{\partial t} \, \theta(t - t_w)$$

holds and implies

$$\chi_{AB}(t - t_w) \equiv \int_{t_w}^{t} dt' \, R_{AB}(t, t') = \frac{1}{2k_B T} [\Delta_{AB}(t - t_w) - \Delta_{AB}(0)]$$

Brownian motion



First example of dynamics of an *open system*

The system : the Brownian particle

The bath : the liquid

Interaction : collisional or potential

'Canonical setting'

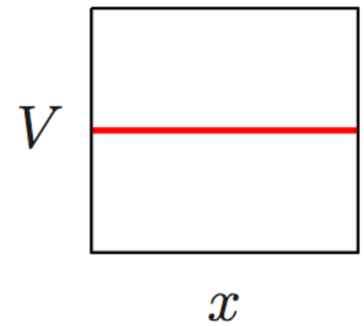
A few Brownian particles or tracers ● imbedded in, say, a molecular liquid.

Late XIX, early XX (Brown, Einstein, Langevin)

Fluctuation-dissipation

Brownian motion

$$m\dot{v} + \gamma v = h + \eta$$



Correlation $\langle x(t)x(t_w)\rangle_{h=0} \mapsto 2\frac{k_BT}{\gamma}\ \min(t, t_w)$ at $t, t_w \gg t_I$ ~~Stationary~~

Displacement $\langle [x(t) - x(t_w)]^2\rangle_{h=0} \mapsto 2\frac{k_BT}{\gamma}\ (t - t_w)$ at $t, t_w \gg t_I$

Linear response $\left.\frac{\delta\langle x(t)\rangle_h}{\delta h(t_w)}\right|_{h=0} = \gamma^{-1}\theta(t - t_w)$

$$2k_BTR_{xx}(t, t_w) = \partial_{t_w}C_{xx}(t, t_w)\,\theta(t - t_w)$$

FDT does not hold

$$2k_BTR_{xx}(t, t_w) = \partial_t\Delta_{xx}(t, t_w)\,\theta(t - t_w)$$

looks like FDT

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Fluctuation-dissipation

Active dumbbell in the last diffusive regime

The c.o.m. diffuses, $\Delta^2_{\rm cm}(t+t_0,t_0) \simeq 2dD_A\, t$, for $t \gg t_a$,

with the diffusion constant $D_A = k_BT/(2\gamma)\,(1+\text{Pe}^2)$

The c.o.m. integrated linear response function $\chi_{\rm cm}(t+t_0,t_0) = d\mu\, t$

with the mobility $\mu = 1/(2\gamma)$

We use the deviation from equilibrium fluctuation-dissipation theorem,

$$\boxed{\chi_{\rm cm}(t+t_0,t_0) = 2k_BT_{\rm eff}(t+t_0,t_0)\Delta^2_{\rm cm}(t+t_0,t_0)}$$

to define, a possibly time(s)-dependent, effective temperature, $T_{\rm eff}$.

For the active dumbbell, at $t > t_a$, we find a constant

$$\boxed{k_BT_{\rm eff} = \frac{\mu}{D_A} = k_BT\,\left(1+\frac{\text{Pe}^2}{8}\right)}$$

Fluctuation-dissipation

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with the diffusion constant $D_A = k_BT/(2\gamma)\,(1+\text{Pe}^2)$

The c.o.m. integrated linear response function $\chi_{\rm cm}(t+t_0,t_0) = d\mu\, t$

with the mobility $\mu = 1/(2\gamma)$ implying

$$k_BT_{\rm eff} = \frac{\mu}{D_A} = k_BT\,\left(1+\frac{\text{Pe}^2}{8}\right)$$

Exercise: Prove these results.

Fluctuation-dissipation

Active dumbbell

The definition of the effective temperature using the deviation from the equilibrium fluctuation-dissipation theorem

$$\boxed{\chi_{\rm cm}(t+t_0,t_0) = 2k_B T_{\rm eff}(t+t_0,t_0)\Delta^2_{\rm cm}(t+t_0,t_0)}$$

is not equivalent to the kinetic temperature

$$\boxed{k_B T_{\rm kin}(t_0) = 2m_{\rm d}\langle v^2_{{\rm cm}\,a}(t_0)\rangle}$$

- The kinetic temperature concerns the velocity variable while the effective temperature concerns the position variable.
- The kinetic temperature is an instantaneous measurement while the effective temperature is a time-delayed measurement.

Fluctuation-dissipation

Active dumbbell

The definition of the effective temperature using the deviation from the equilibrium fluctuation-dissipation theorem yields

$$k_B T_{\rm eff} = k_B T \left(1 + \mathrm{Pe}^2/8\right)$$

and is not equivalent to the kinetic temperature

$$k_B T_{\rm kin} = k_B T \left[1 + m_{\rm d} k_B T/(2\gamma\sigma_{\rm d})^2 \, \mathrm{Pe}^2\right]$$

- The kinetic temperature concerns the velocity variable while the effective temperature concerns the position variable.
- The kinetic temperature is an instantaneous measurement while the effective temperature is a time-delayed measurement.

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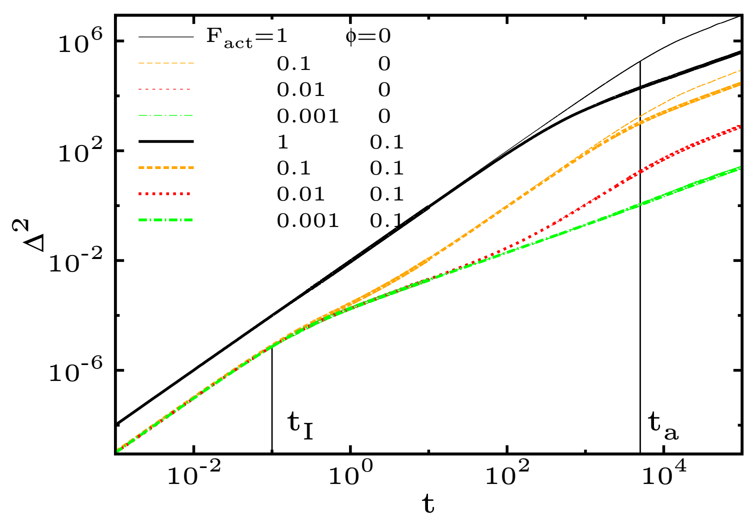
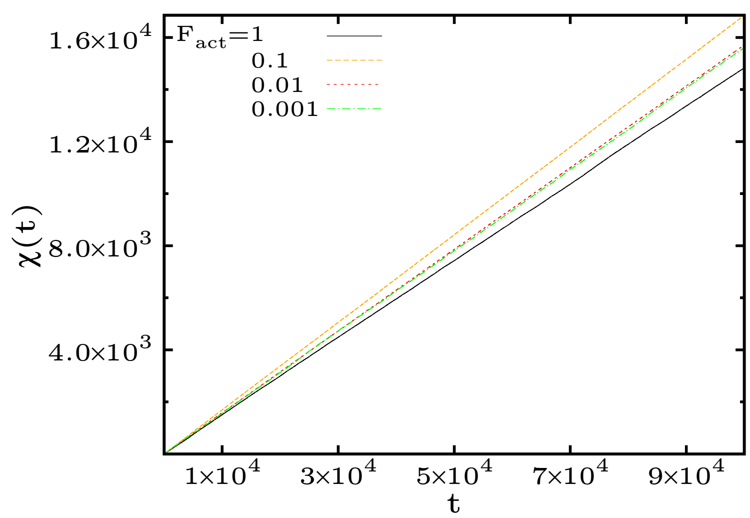
Fluctuation-dissipation

Active finite (low) density dumbbell system

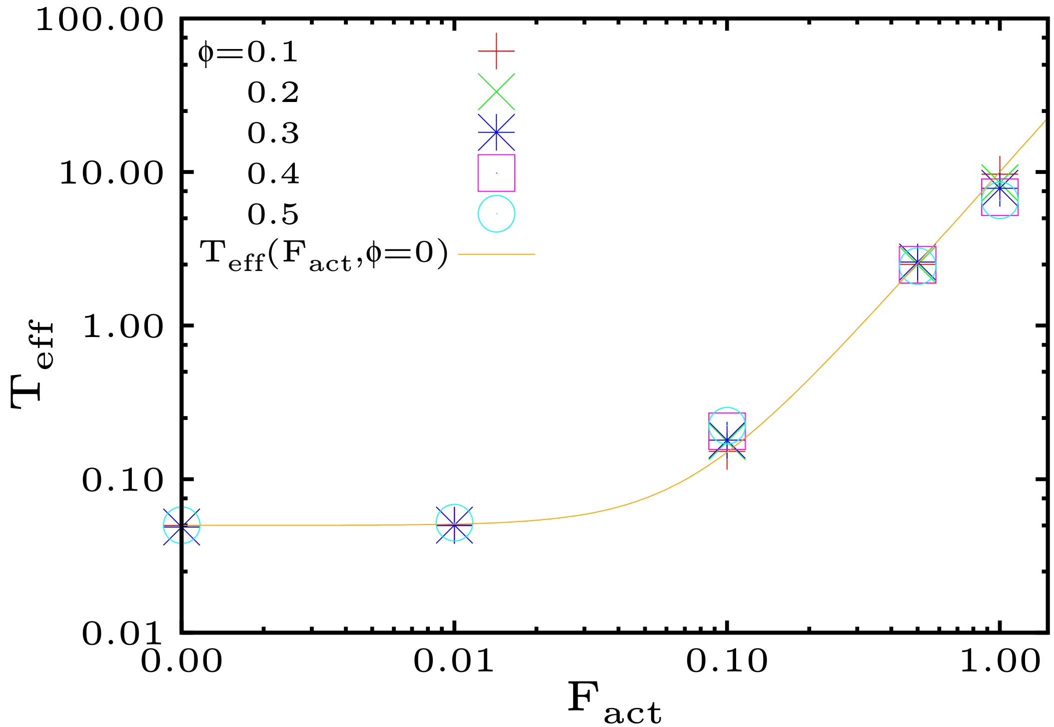
$\phi = 0.1$





Fluctuation-dissipation

$$\chi_{\rm cm}(t+t_0,t_0) = 2k_B T_{\rm eff}\, \Delta^2_{\rm cm}(t+t_0,t_0)$$



$T_{\rm eff} \simeq 200\, T$

$T = 0.05$

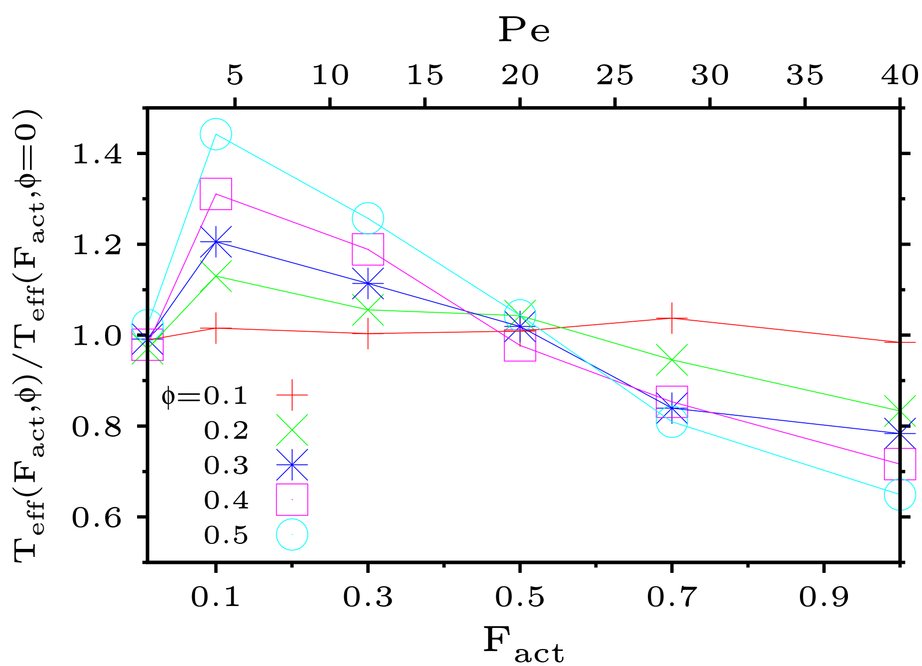
Pe $\simeq 4$ Pe $\simeq 40$

Very weak ϕ-dependence in this scale but...

Fluctuation-dissipation

$$\chi_{\rm cm}(t+t_0,t_0) = 2k_B T_{\rm eff}\, \Delta^2_{\rm cm}(t+t_0,t_0)$$

Non monotonic dependence on ϕ



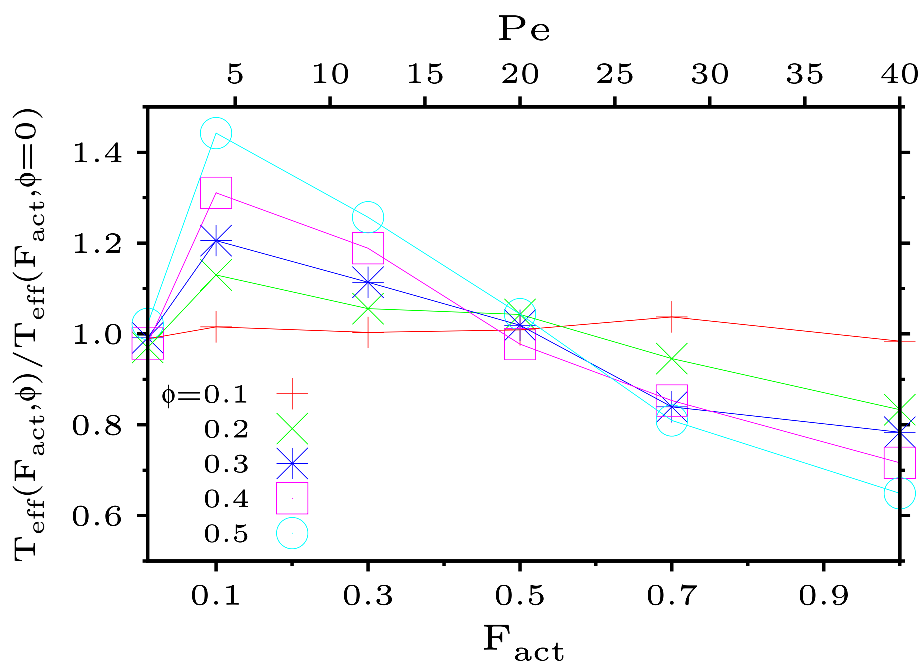
"Dynamics of a homogeneous active dumbbell system",

Suma, Gonnella, Laghezza, Lamura, Mossa & LFC, Phys. Rev. E 90, 052130 (2014)

Fluctuation-dissipation

$$\chi_{\rm cm}(t+t_0,t_0) = 2k_B T_{\rm eff}\, \Delta^2_{\rm cm}(t+t_0,t_0)$$

Like in **Wu & Libchaber** Differently



"Dynamics of a homogeneous active dumbbell system",

Suma, Gonnella, Laghezza, Lamura, Mossa & LFC, Phys. Rev. E 90, 052130 (2014)

Effective temperature

Properties and measurement

— Relation to entropy.

— Control of heat-flows : ΔQ follows ΔT.

— Partial equilibration – transitivity :

$T_A = T_B, T_B = T_C \Rightarrow T_A = T_C$.

thermometers for systems in

good thermal contact (ΔQ)

Review LFC 11

Whatever we identify with a temperature should have these properties

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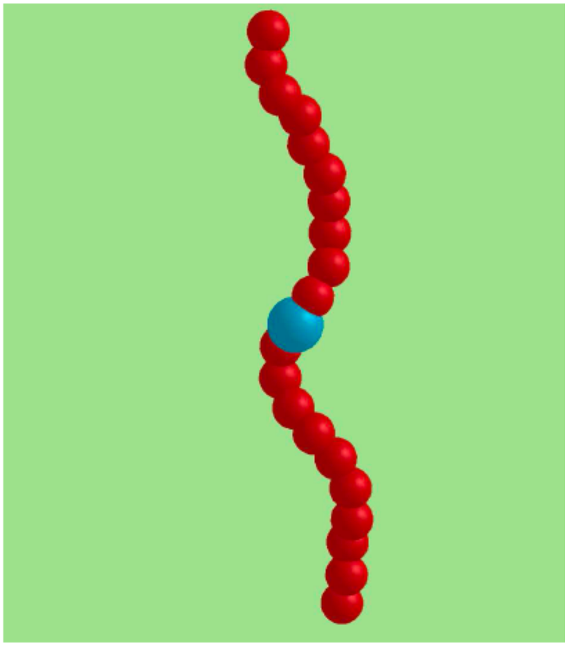
Interacting polymers

The “DNA” example



Molecular dynamics

Linear molecules

$\mathbf{F}_i^{\mathrm{det}}$ deterministic force

$\mathbf{F}_i^{\mathrm{act}}$ stochastic motor forces

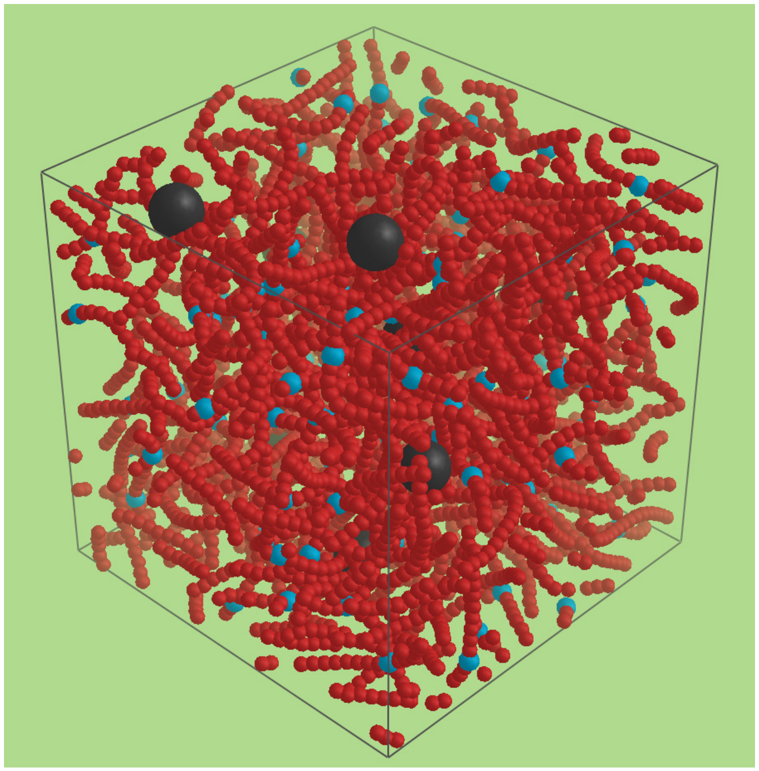
act during τ

$$m\dot{\boldsymbol{v}}_i + \gamma \boldsymbol{v}_i = \mathbf{F}_i^{\mathrm{det}}(\{\boldsymbol{r}_j\}) + \mathbf{F}_i^{\mathrm{act}} + \boldsymbol{\eta}_i$$

Loi, Mossa & LFC 08-11

Interacting polymers

The "DNA" example



Molecular dynamics

Linear molecules

$\mathbf{F}_{ia}^{\rm det}$ deterministic force

$\mathbf{F}_{ia}^{\rm act}$ stochastic motor forces

act during τ

on $\%$ polymers

Passive tracers

$$m\dot{\boldsymbol{v}}_{ia} + \gamma \boldsymbol{v}_{ia} = \mathbf{F}_{ia}^{\rm det}(\{\boldsymbol{r}_j\}) + \mathbf{F}_{ia}^{\rm act} + \boldsymbol{\eta}_{ia}$$

Loi, Mossa & LFC 08-11

Interacting polymers

Forces

$$\mathbf{F}_{\alpha i}^{\rm det} = -\sum_{\nu(\neq\alpha)}^{N_p}\sum_{j=1}^{N_m}\boldsymbol{\nabla}_{\nu j}V_{\rm inter}(r_{\alpha i\nu j}) - \sum_{j=1}^{N_m}\boldsymbol{\nabla}_{\nu j}V_{\rm intra}(r_{\alpha i\nu j})$$

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

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

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

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

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

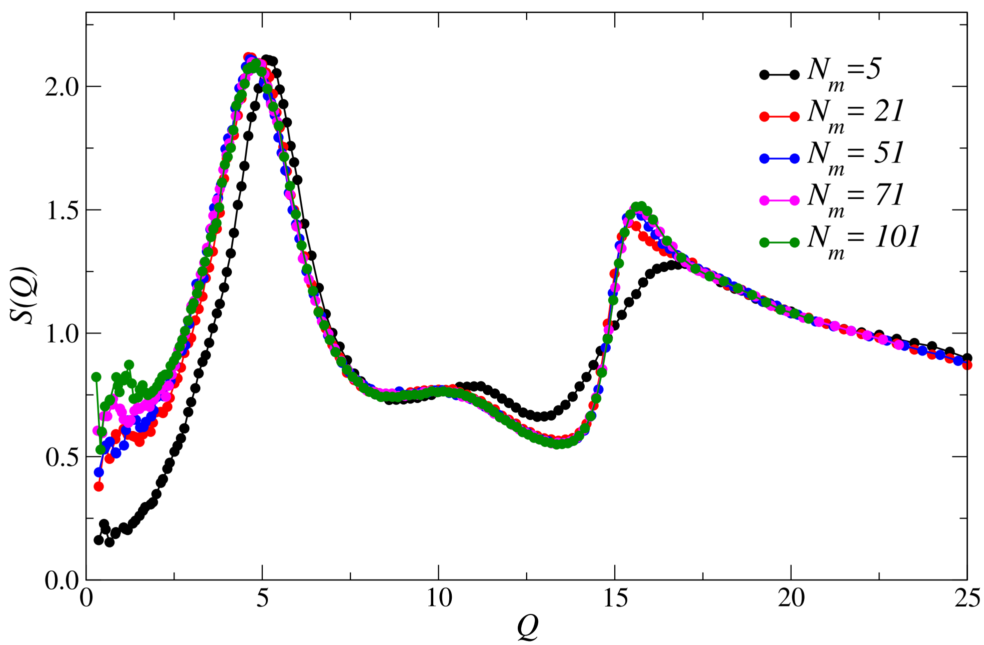
Interacting polymers

Structure of the passive model : liquid

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 $\alpha \neq \nu$)

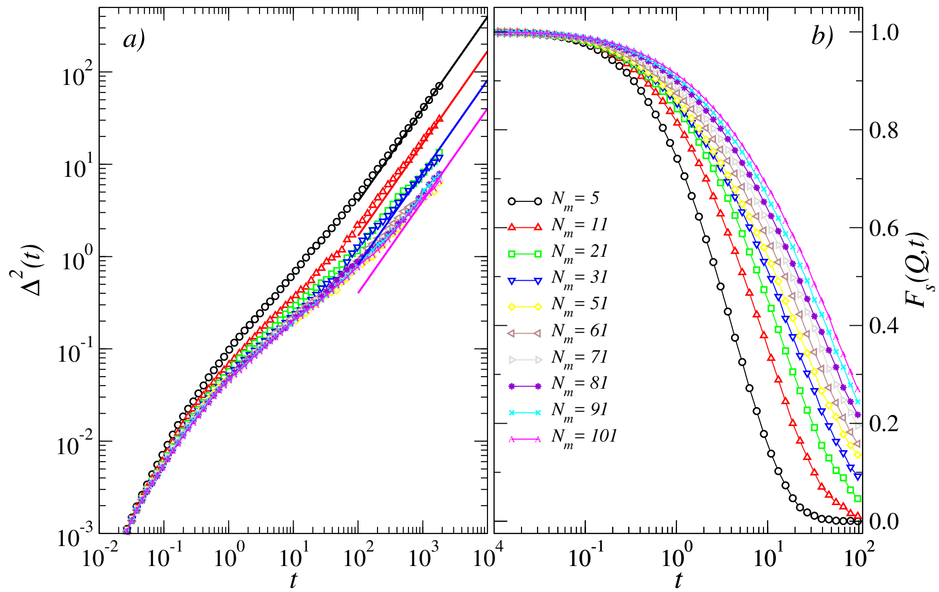
2nd peak

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

Analysis of radius of gyration : non-Gaussian chains.

Interacting polymers

Dynamics of the passive model : liquid



$D \simeq N_m^{-1}$

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

for

$N_m \lesssim 50$

We used

$N_m = 21$

$$\Delta^2(t) = \frac{1}{N_p N_m} \sum_{\alpha=1}^{N_p} \sum_{i=1}^{N_m} \langle |\boldsymbol{r}_{\alpha i}(t+t_0) - \boldsymbol{r}_{\alpha i}(t_0)|^2 \rangle$$ Mean-square displacement

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

Interacting polymers

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

$$|\mathbf{F}_{\alpha i}^{\mathrm{act}}| = f \, \frac{1}{N_p N_m} \sum_{\alpha=1}^{N_p} \sum_{i=1}^{N_m} |\mathbf{F}_{\alpha i}^{\mathrm{det}}| = f \, \overline{F} \qquad \overline{F} \simeq 163.5$$

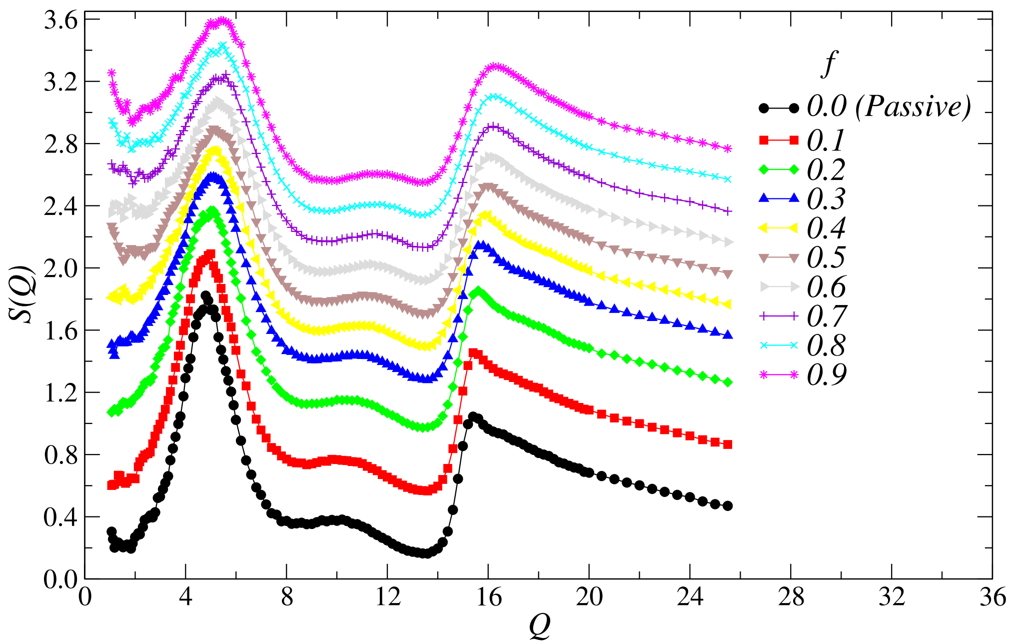
– Time series of randomly applied kicks on % polymers.

– Activation time scale $\tau = 500$ MDs: constant $\mathbf{F}_{\alpha i}^{\mathrm{act}}$ over this period.

The motor action is independent of the structural rearrangements induced

Interacting polymers

Structure properties



1st peak $\rightarrow$ right :

nn dist. decreases, *i.e.*

crowding.

Width increases &

height decreases, *i.e.*

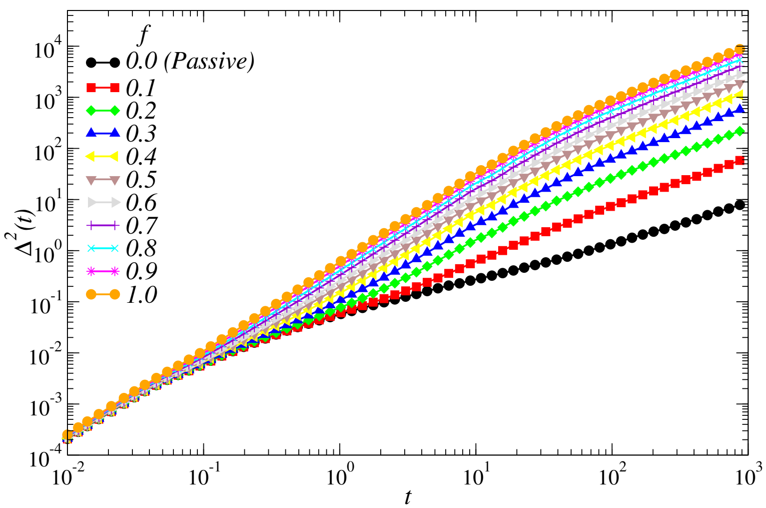
disorder.

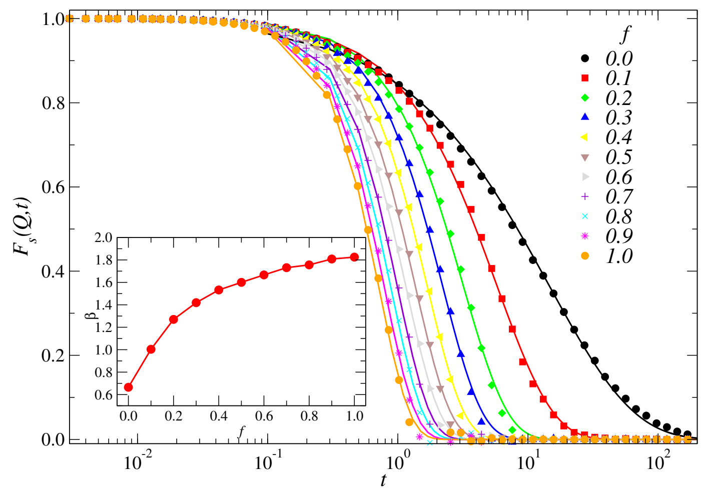
Averaged radius of gyration decreases with increasing f : chain folding.

Complex dependence of its pdf with f.

Interacting polymers

Dynamics: the diffusion constant increases with Pe





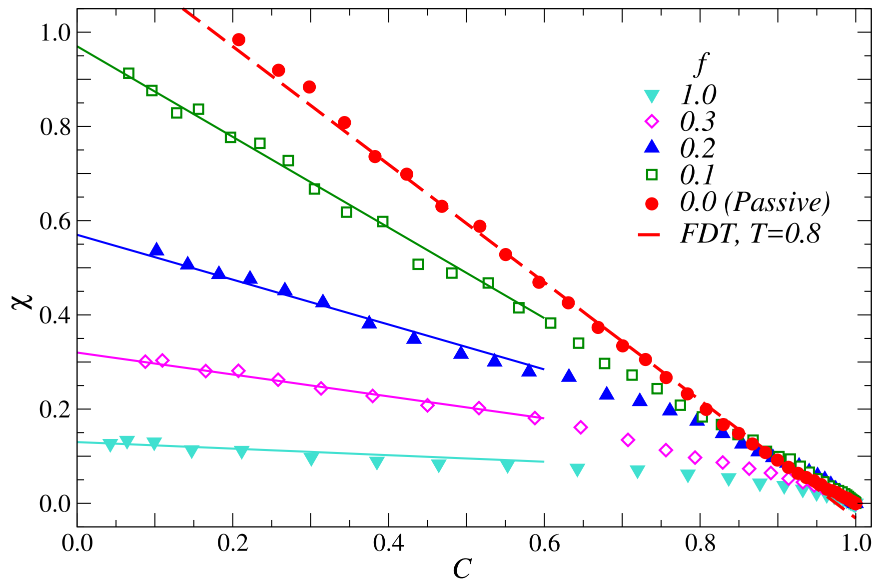
$$D_A/D \simeq 1{+}1423\, f^{2.29}$$

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

Could the exponent be actually 2 and $D_A/D \simeq 1 + c\,\mathrm{Pe}^2$ as for the dumbbell system

Active matter

Integrated linear response against correlation function



q_0 first peak in structure factor

$$C(t) \propto \sum \langle e^{i\boldsymbol{q}_0 \cdot [\boldsymbol{r}(t+t_0,t_0) - \boldsymbol{r}(t_0)]} \rangle$$

$$\chi(t) \propto \sum \int_{t_0}^{t+t_0} dt' \left. \frac{\delta \langle e^{i\boldsymbol{q}_0 \cdot \boldsymbol{r}(t+t_0)} \rangle}{\delta h(t')} \right|_{h=0}$$

$$H \to H - 2h \sum \epsilon \cos(\boldsymbol{q}_0 \cdot \boldsymbol{r})$$

Sums over all monomers, t is time-delay

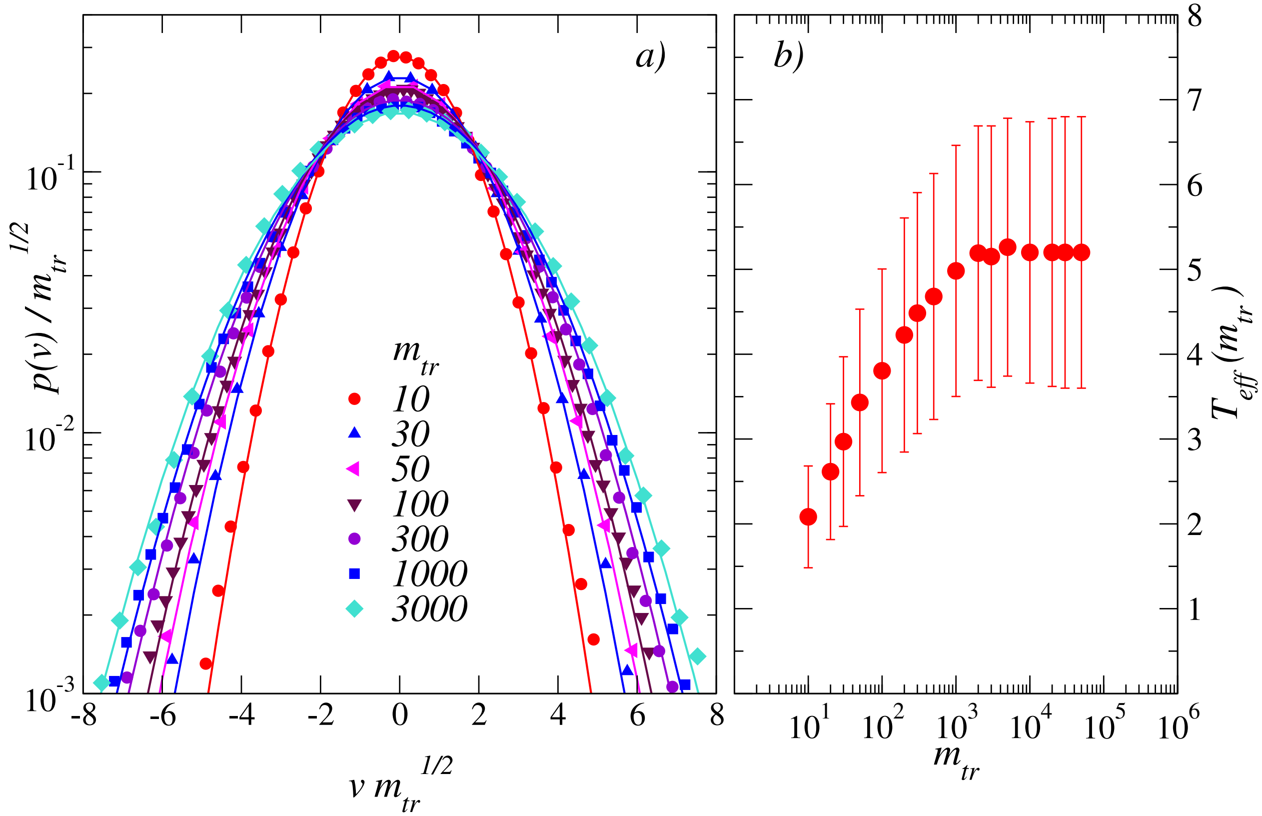
$$\chi(t) = \frac{1}{k_B T_{\rm eff}(t)} [C(0) - C(t)]$$

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

Interacting polymers

Tracer's velocities

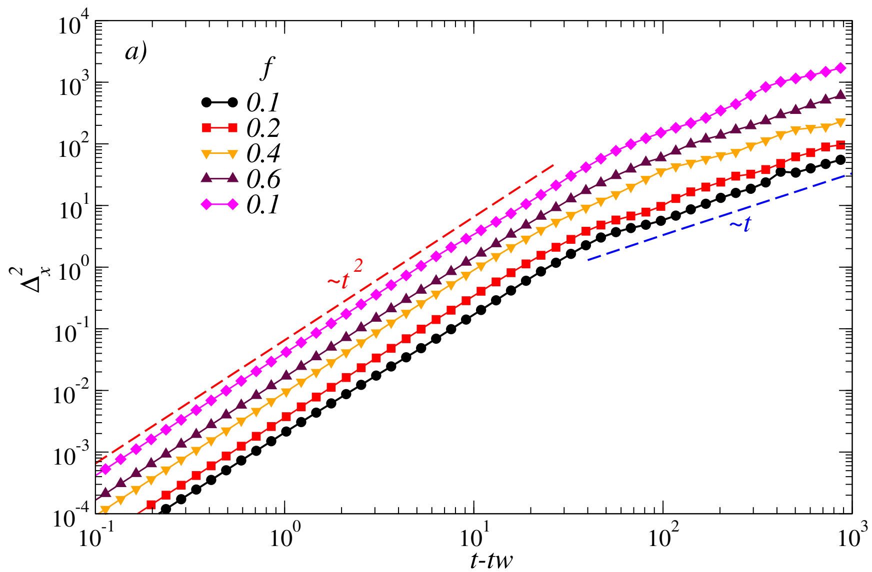
Spherical particles with mass $m_{\rm tr}$ that interact with the active matter.

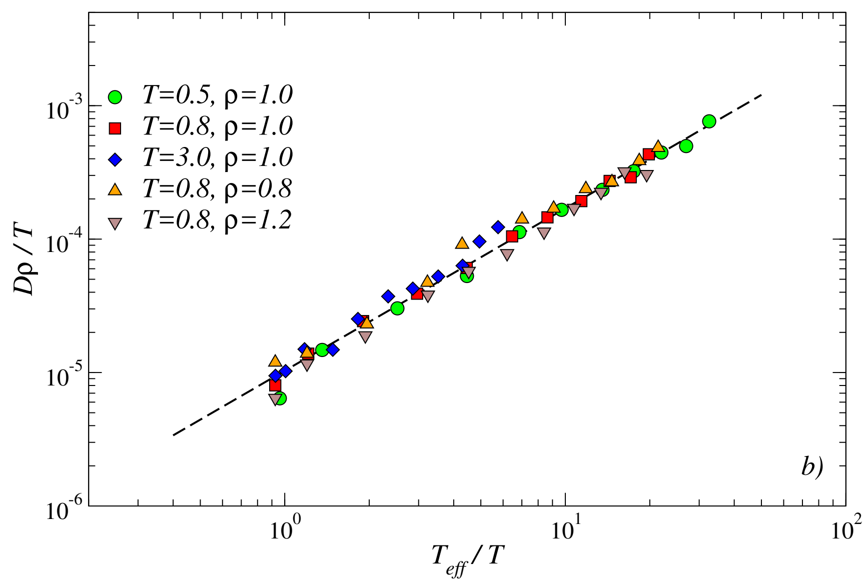


Maxwell pdf of tracers' velocities v at an effective temperature $T_{\rm eff}(m_{\rm tr})$.

Interacting polymers

Tracer's diffusion (cfr. Wu & Libchaber's work)



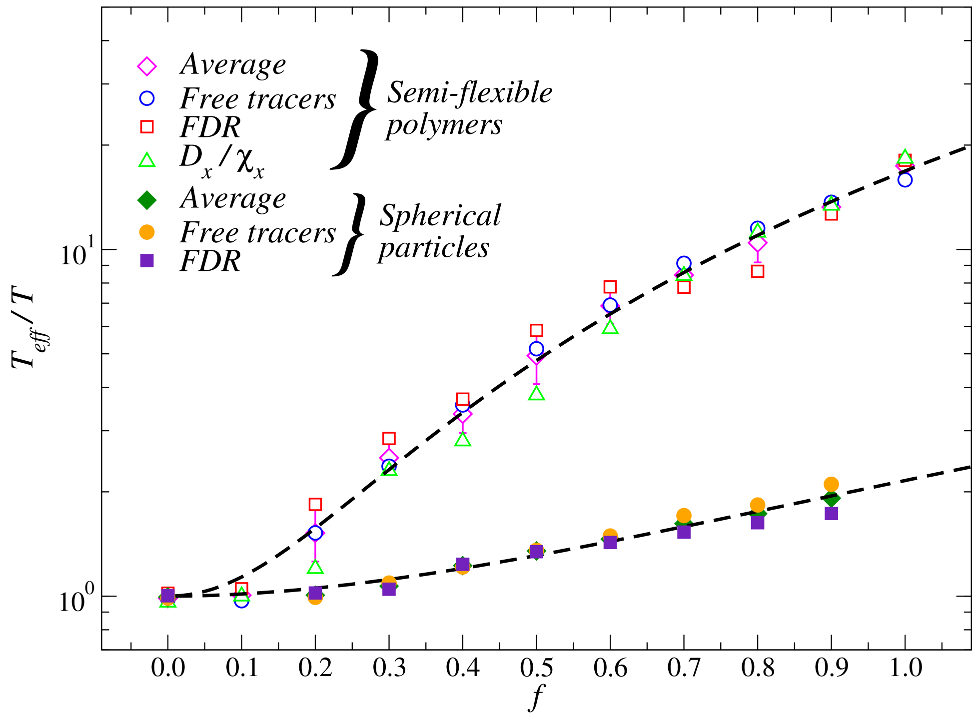


$$\Delta^2_{\rm tr}(t+t_0,t_0) = \langle [\boldsymbol{r}(t+t_0) - \boldsymbol{r}(t_0)]^2 \rangle \simeq 2dDt$$

Brownian motion : $D \propto k_B T$ **in active matter** $D_{\rm eff} \propto k_B T_{\rm eff}$

Interacting polymers

Outcome of FDT on polymers & tracers' diffusion and kinetic energy

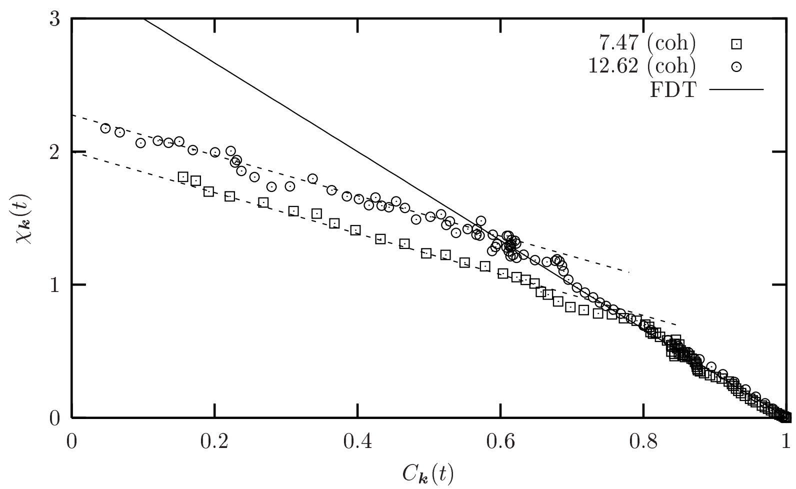


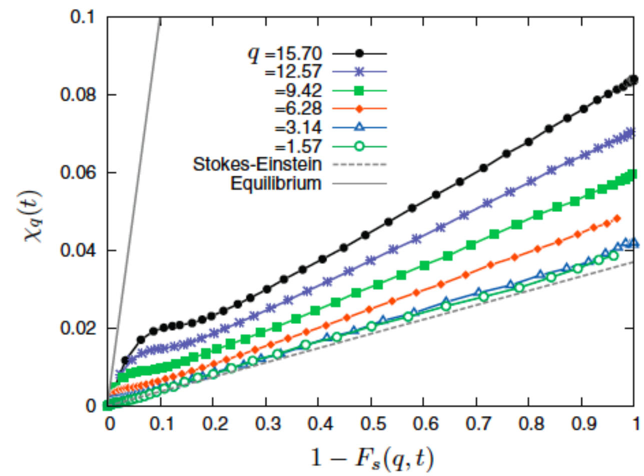
$$\boxed{T_{\rm eff}/T \simeq 1 + c\, f^2} \qquad \stackrel{?}{=} \qquad 1 + c\, \mathsf{Pe}^2$$

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

Partial equilibrations

Wave-vector dependence analysis





Lennard-Jones binary mixture

Berthier & Barrat 00

Fine

Active disks

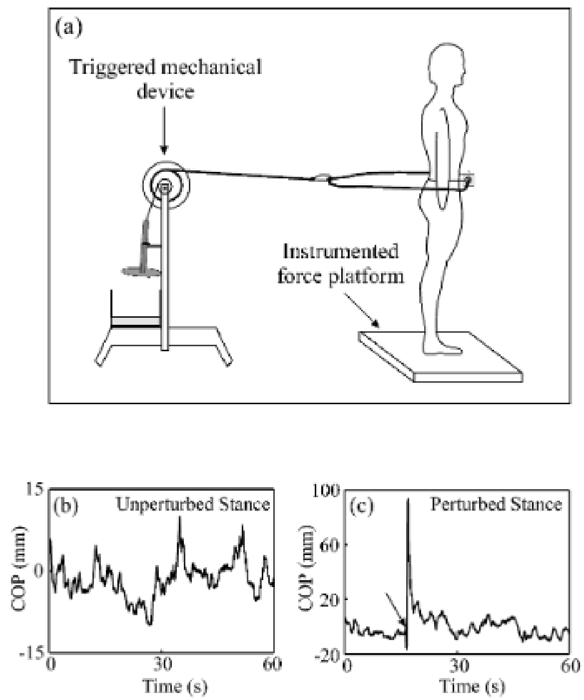
Levis & Berthier 15

Problems

To be further studied

Experiments

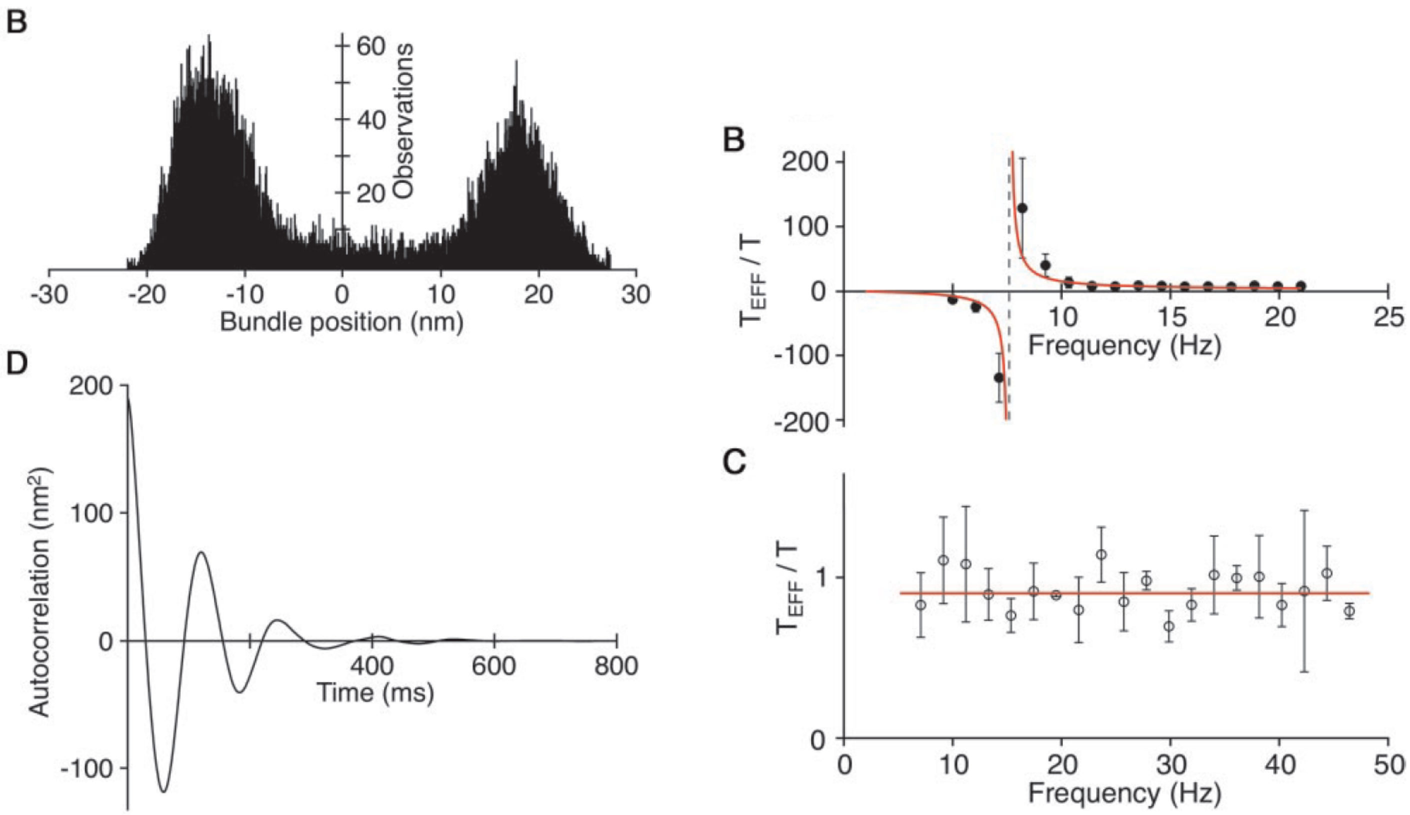
Human FDT



"Human Balance out of Equil. : Nonequilibrium Statistical Mechanics in Posture Control", **Lauk, Chow, Pavlik & Collins, Phys. Rev. Lett. 80, 413 (1998)**

Experiments

Ear Hair bundle

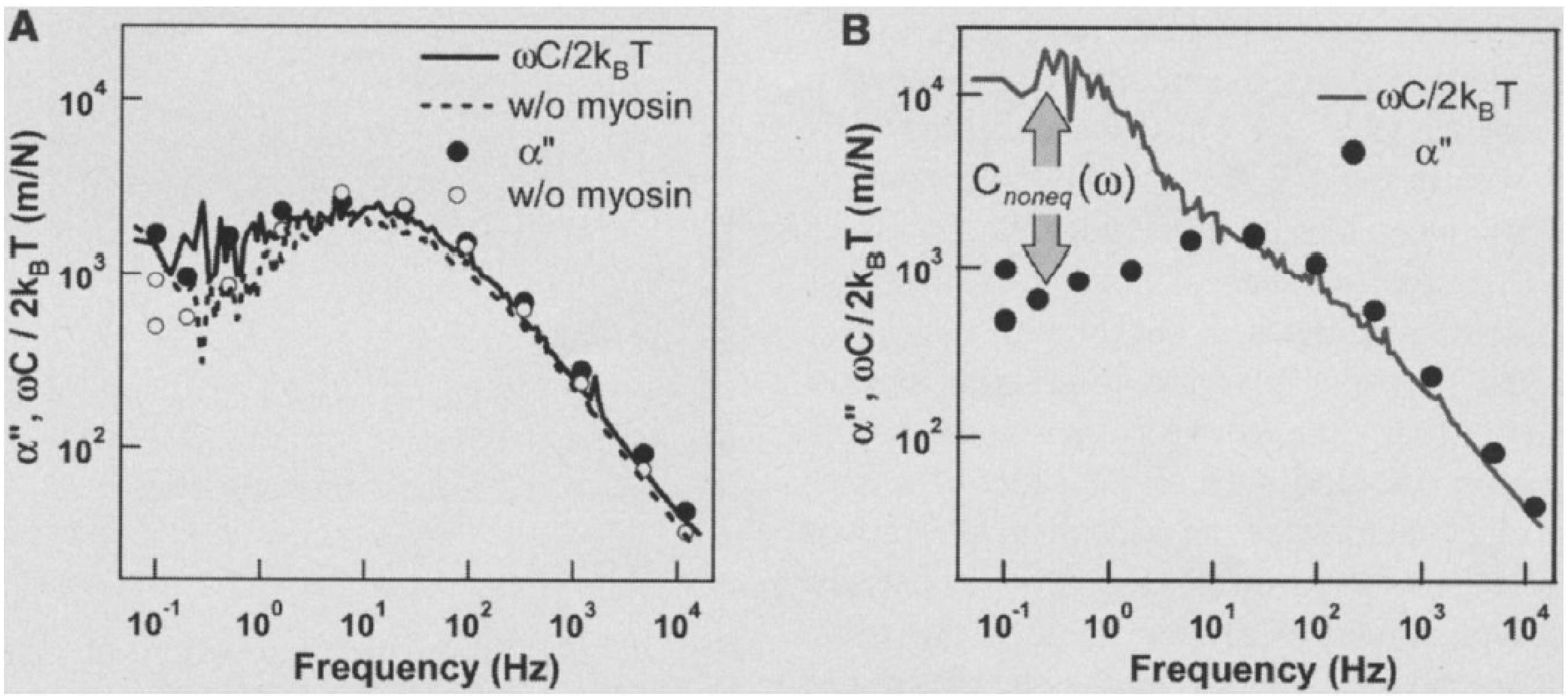


"Comparison of a hair bundle's spontaneous oscillations with its response to mechanical stimulation reveals the underlying active process"

Martin, Hudspeth & Jülicher, PNAS 98, 14380 (2001)

Experiments

Mechanical response of the cell cytoskeleton



"Non equilibrium mechanics of active cytoskeletal network"

Mizuno, Tardin, Schmidt, MacKintosh, Science 315, 370 (2015)

Experiments

Boltzmann distribution for the sedimentation of a gas

Under the only effect of gravity, how does the density of a perfect gas depend upon the vertical distance z from a reference z_0?

$$P(z+dz) - P(z) = -mg\rho(z)\,dz \quad \Rightarrow \quad \frac{dP(z)}{dz} = mg\rho(z)$$

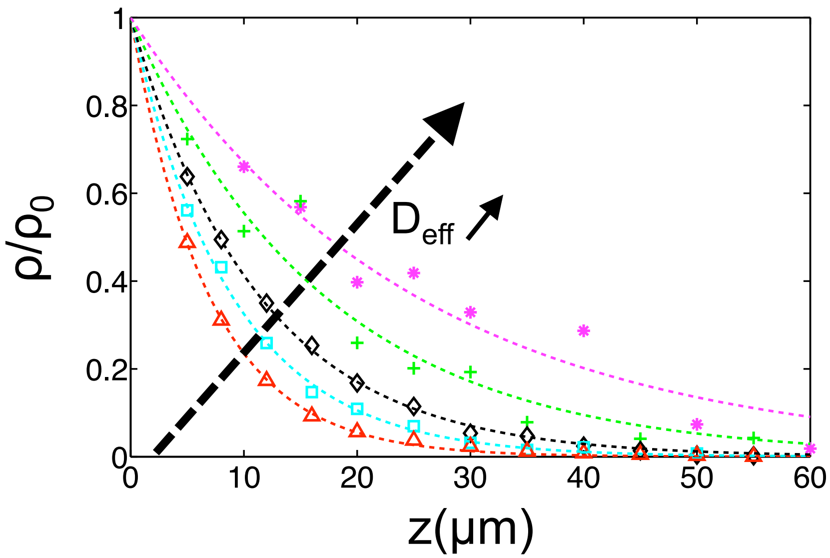
with m the mass of the particles in the gas, g the gravitational acceleration, $\rho(z)$ the density of the gas at height z and $P(z)$ its pressure at the same height.

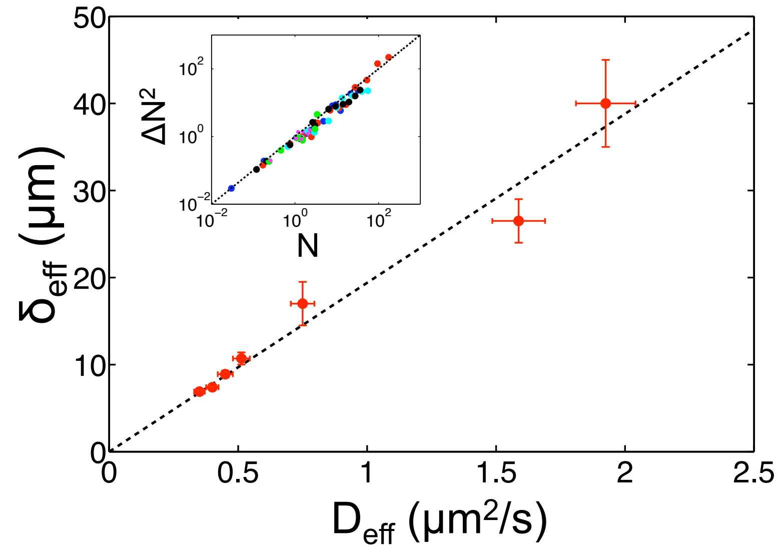
Using the perfect gas law $P(z) = \rho(z)k_B T$

$$\frac{d\rho(z)}{dz} = -\frac{mg}{k_B T}\,\rho(z) \quad \Rightarrow \quad \boxed{\rho(z) = \rho(z_0)\,e^{-\beta mgz}}$$

Experiments

Sedimentation of Janus particles in a very dilute limit





$$\rho(z) \simeq \rho_0 \, e^{-z/\delta_{\text{eff}}} \quad \text{with} \quad \delta_{\text{eff}} = \frac{k_B T_{\text{eff}}}{mg} \propto D_{\text{eff}}$$

"Sedimentation and effective temperature of active colloidal suspensions"

Palacci et al. Phys. Rev. Lett. 105, 088304 (2010)

Summary

- Deviations from FDT reveal the nonequilibrium character of a system.
- It was used for ear hair bundles, the cytoskeleton, bacterial baths, etc.
- A time-delay dependent effective temperature can be extracted from the modification of the FDT.
- Its thermodynamic properties have to be tested by measuring it with thermometers, checking partial equilibrations, etc.
  - In low density interacting systems of particles and polymers under adamant motors (homogeneous liquid systems) ✓
  - In interacting active dumbbell systems : need to revisit the effects of clustering and coexistence (see next lectures !)
  - In active hard disk models : same claim as above.
  - In Vicsek model : + difficulty posed by singular passive limit.