Nonlinear response and fluctuations of a driven tracer particle in simple model fluids

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degli Studi
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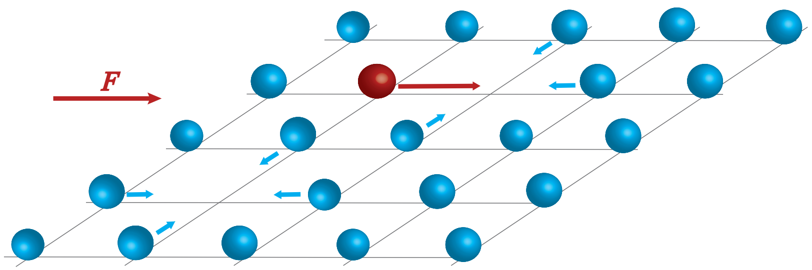
Outline of the talk

- Driven tracer particle in a lattice gas

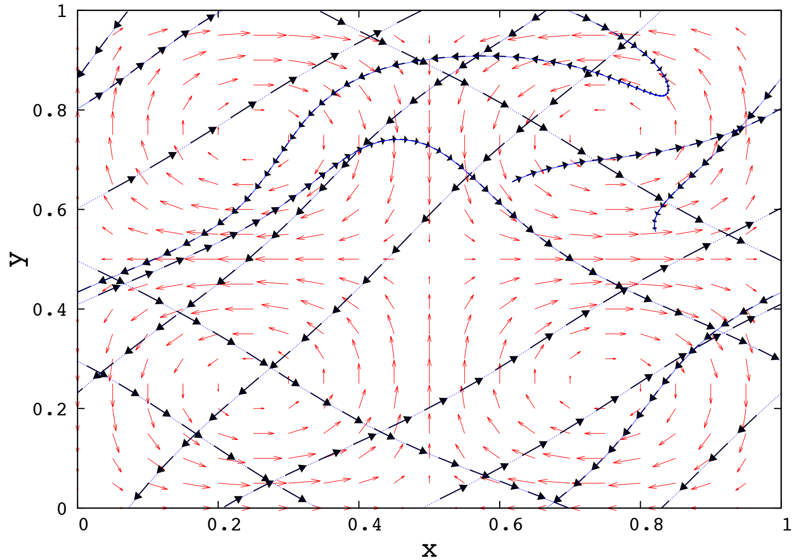
In collaboration with
O. Bénichou, P. Illien,
G. Oshanin, R. Voituirez
Université Pierre et Marie Curie, Paris 6



PRL (2014), PRE (2016), PRL (2018), JPCM (2018)

- Nonlinear response of an inertial particle in a steady flow

In collaboaration with
Fabio Cecconi, Andrea Puglisi
and Angelo Vulpiani
ISC-CNR, Univ. Sapienza, Roma



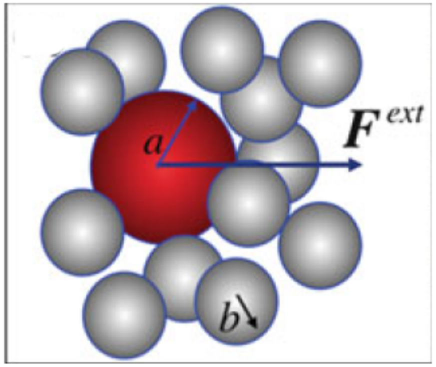
PRL (2016), EPJE (2017), JPCM (2018)

Nonlinear response of a driven tracer

Rheological properties in soft matter from the microscopic motion of colloidal tracers

Puertas & Voigtmann (2014), Squires & Mason (2010)

Active microrheology: tracer particle (TP) driven by an external force F



Applications: complex fluids, gels, glasses, living cells, granular systems,…

→ Characteristic curve: Force-Velocity relation, V vs F

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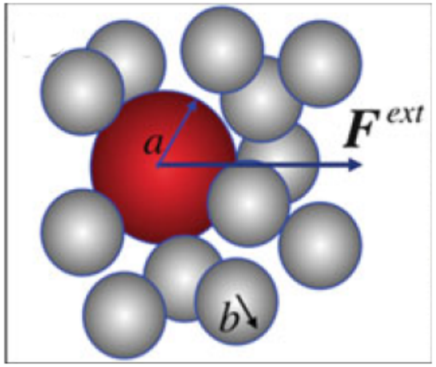
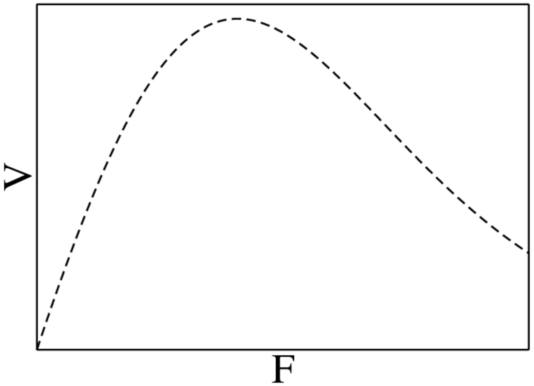


Applications: complex fluids, gels, glasses, living cells, granular systems,…

→ Characteristic curve: Force-Velocity relation, V vs F

Nonlinear response regime: increasing the applied force can reduce the probe's drift velocity in the force direction

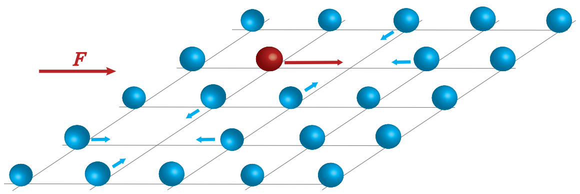
→ Negative differential mobility



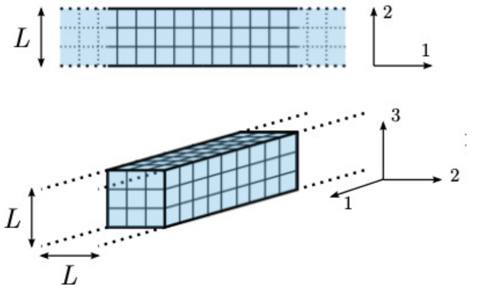
Driven tracer in a hard-core lattice gas

(N-1) hard-core particles,
symmetric exclusion process,
average waiting time τ^*

Infinite lattice



Confined geometries



Tracer driven by a force F
asymmetric exclusion process,
average waiting time τ

Density $\rho = \dfrac{N}{V}$

Tracer jump probabilities, local detailed balance $p_\nu = \dfrac{e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\nu}}{\sum_\mu e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\mu}}$

$\nu = \pm 1, \ldots, \pm d \quad \boldsymbol{F} = F\boldsymbol{e}_1$

Force-velocity relation?

Decoupling approximation and analytic solution

Master Equation for $P(\boldsymbol{R}_{TP}, \eta; t)$

$\boldsymbol{R}_{TP}$ tracer position

η obstacle configuration

$$\partial_t P(\mathbf{R}_{TP}, \eta; t) = \mathcal{L}_{\mathrm{bath}} P + \mathcal{L}_{\mathrm{TP}} P$$

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Decoupling approximation

$$\langle \eta(\boldsymbol{R}_{TP} + \boldsymbol{\lambda})\eta(\boldsymbol{R}_{TP} + \boldsymbol{e}_\nu)\rangle \approx \langle \eta(\boldsymbol{R}_{TP} + \boldsymbol{\lambda})\rangle\langle \eta(\boldsymbol{R}_{TP} + \boldsymbol{e}_\nu)\rangle$$

for $\boldsymbol{\lambda} \neq \boldsymbol{e}_\nu$

$$V(F) \equiv \frac{d\langle \boldsymbol{R}_{TP} \cdot \boldsymbol{e}_1\rangle}{dt} = \frac{1}{2d\tau^*}(A_1 - A_{-1})$$

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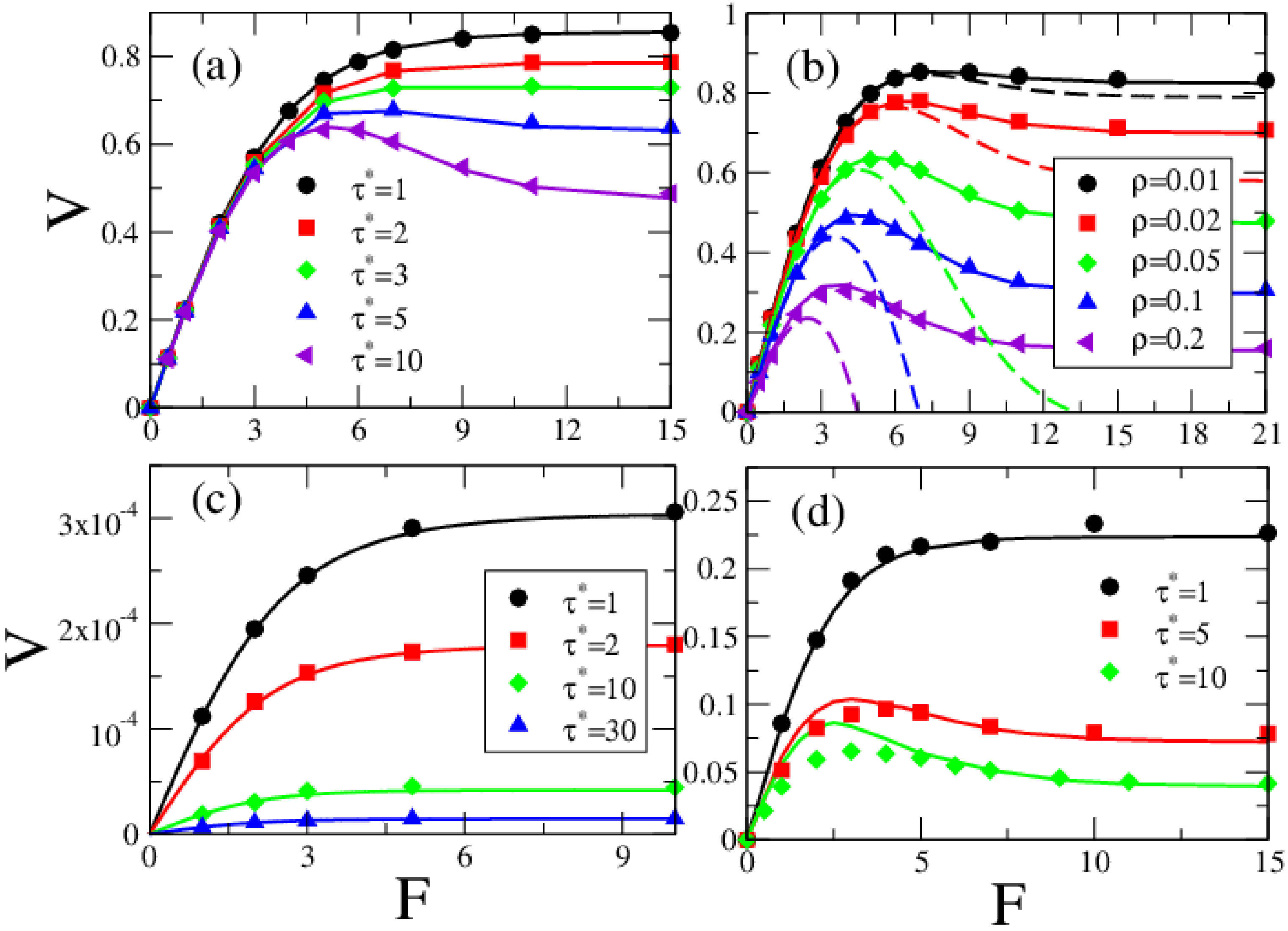
Nonlinear system of equations

$$A_\nu = 1 + \frac{2d\tau^*}{\tau} p_\nu \left[1 - \rho - \rho(A_1 - A_{-1}) \frac{\det C_\nu}{\det C} \right]$$

→ Solution for $V(F)$ for arbitrary values of the parameters

Comparison with Monte Carlo numerical simulations



$d = 2, \tau = 1$

(a) $\rho = 0.05$

(b) $\tau^* = 10$

(c) $\rho = 0.999$

(d) $\rho = 0.5$

→ Good agreement in a wide range of parameters

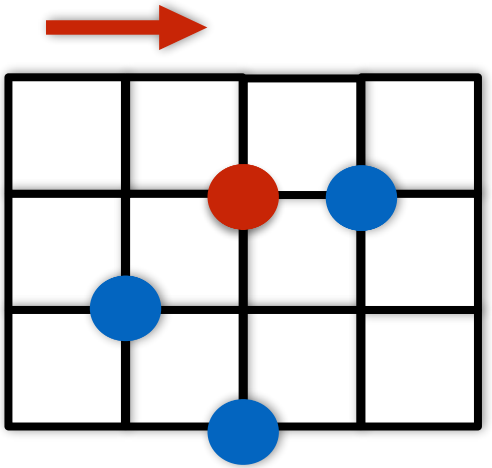
Argument for NDM at low density

$$V(F) = \frac{\text{mean distance}}{\text{mean time of free flight} + \text{mean trapping time}}$$

$$1/\tau_{\text{trap}} = 3/(4\tau^*) + \epsilon/\tau \qquad \epsilon = 2e^{-\beta F/2} \ll 1$$

obstacle steps away

tracer steps in a transverse direction



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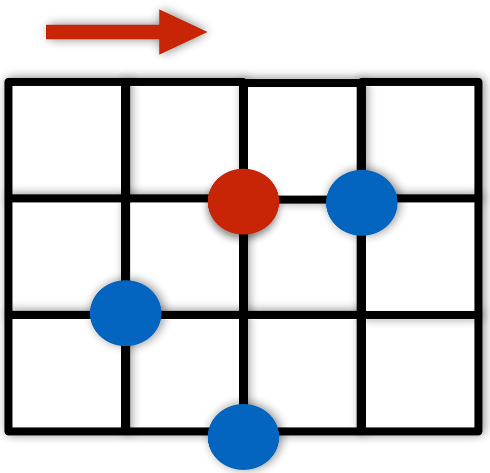


Physical mechanism: a large force

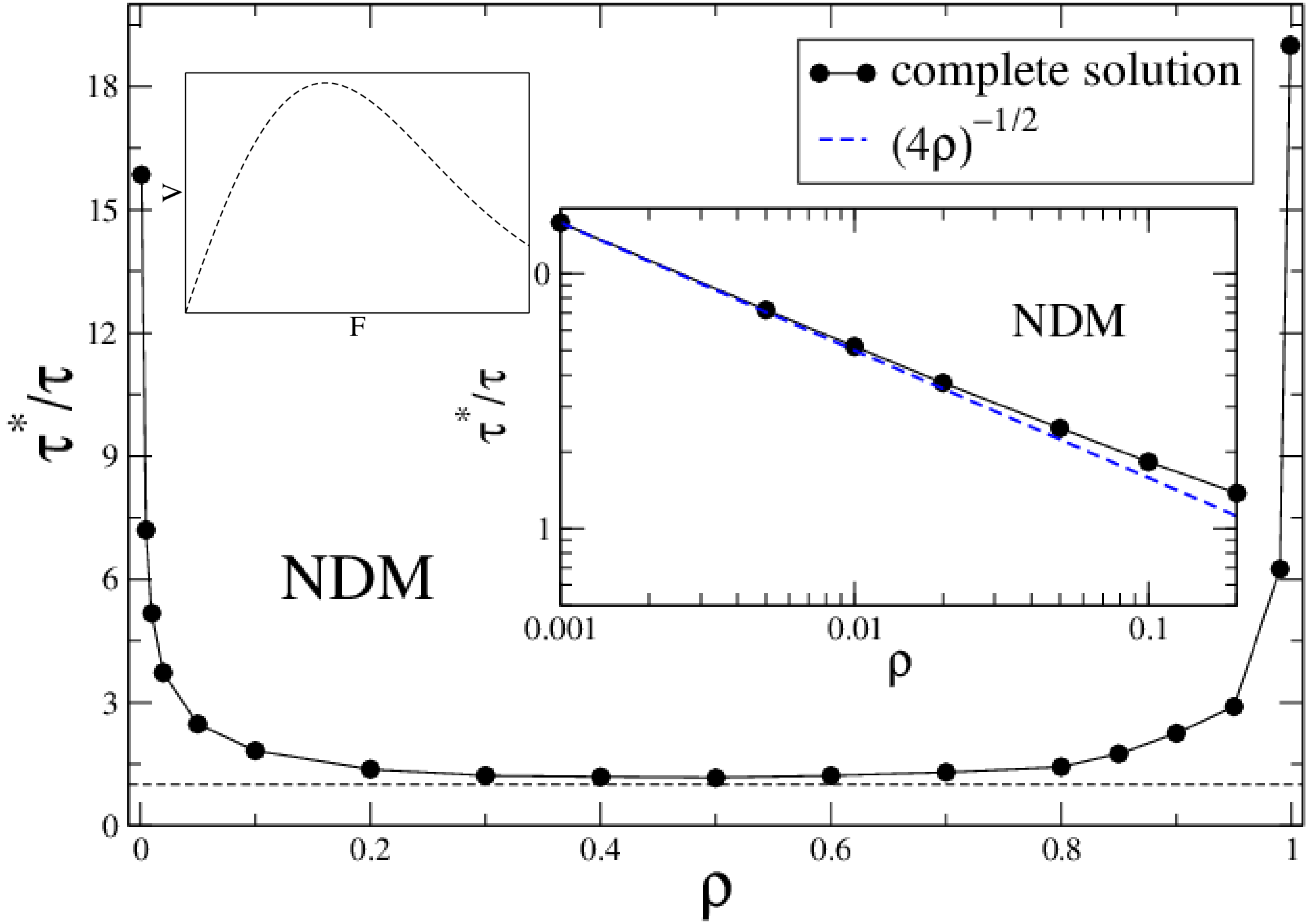
→ reduces the flight time between two consecutive encounters with bath particles;

→ increases the escape time from traps created by surrounding obstacles

For τ^* large enough ("slow" obstacles), traps are sufficiently long lived to slow down the TP when F is increased → NDM

Criterion for negative differential mobility

Parameter space: time scales τ^*/τ and density ρ



Physical mechanism: coupling between density and time scales ratio

Fluctuations and diffusion coefficient

Variance of the tracer

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_X^2(t) = -\frac{2\sigma}{\tau}\left[p_1 \widetilde{g}_{\mathbf{e}_1}(t) - p_{-1}\widetilde{g}_{\mathbf{e}_{-1}}(t)\right] + \frac{\sigma^2}{\tau}\left\{p_1\left[1 - k_{\mathbf{e}_1}(t)\right] + p_{-1}\left[1 - k_{\mathbf{e}_{-1}}(t)\right]\right\}$$

Correlation between tracer and bath particles

$$\widetilde{g}_{\boldsymbol{r}} \equiv \langle (X_t - \langle X_t \rangle)(\eta_{\boldsymbol{r}} - \langle \eta_{\boldsymbol{r}} \rangle)\rangle$$

Diffusion coefficient

$$D \equiv \frac{1}{2d}\lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\sigma_X^2(t)$$

Decoupling approximation

$$\begin{aligned} \langle \eta_{\boldsymbol{r}}\eta_{\boldsymbol{r}'}\rangle &\simeq \langle \eta_{\boldsymbol{r}}\rangle\langle \eta_{\boldsymbol{r}'}\rangle \\ \langle \delta X_t \eta_{\boldsymbol{r}}\eta_{\boldsymbol{r}'}\rangle &\simeq \langle \eta_{\boldsymbol{r}}\rangle\langle \delta X_t \eta_{\boldsymbol{r}'}\rangle + \langle \eta_{\boldsymbol{r}'}\rangle\langle \delta X_t \eta_{\boldsymbol{r}}\rangle \end{aligned}$$

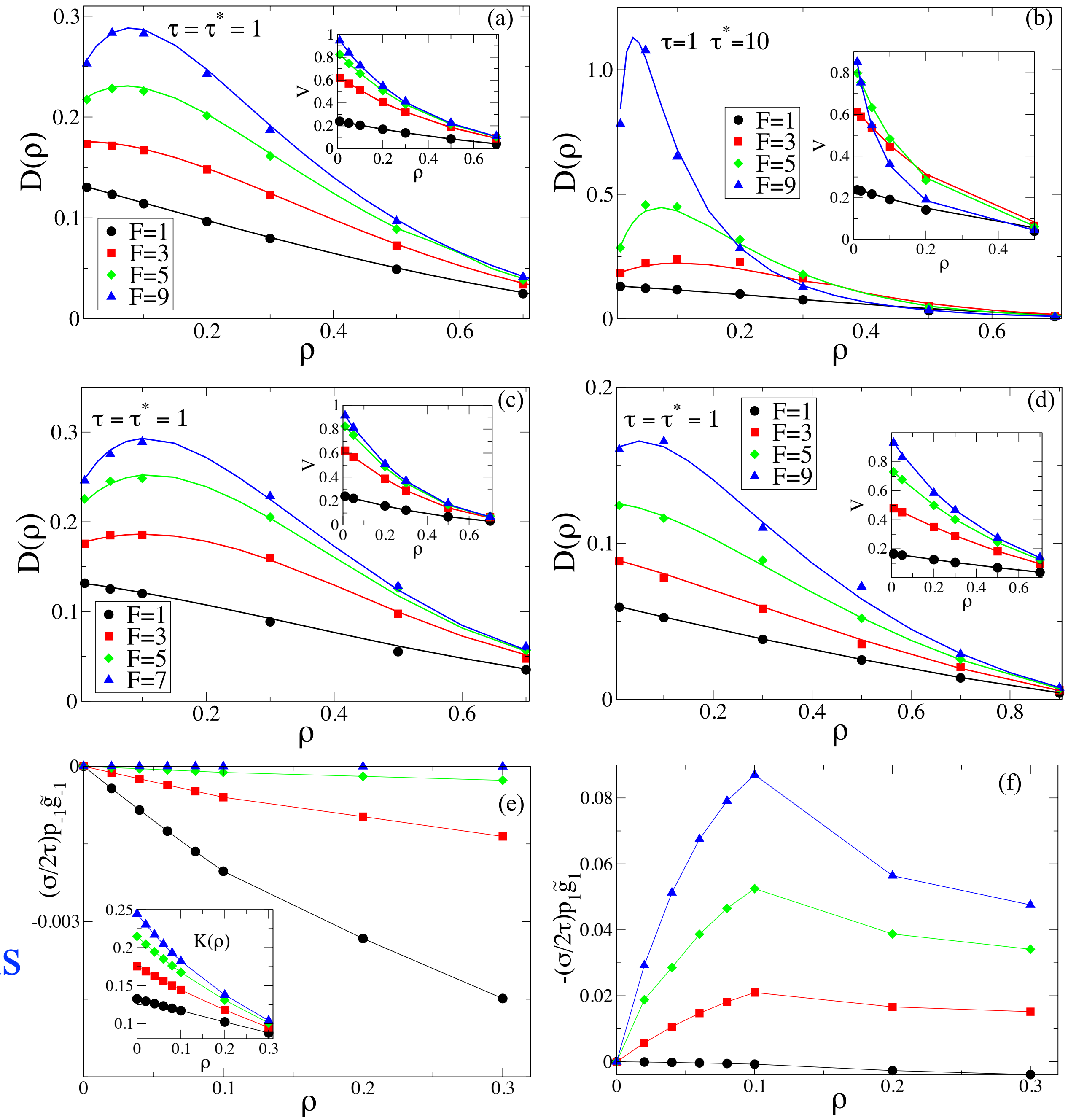
Enhanced diffusivity induced by crowding interactions

2d infinite lattice

Strip-like lattice

3d infinte lattice

cross-correlarions



PART II: nonlinear response of an inertial tracer

Model: inertial tracer in a steady cellular flow, with external force

Thermal noise

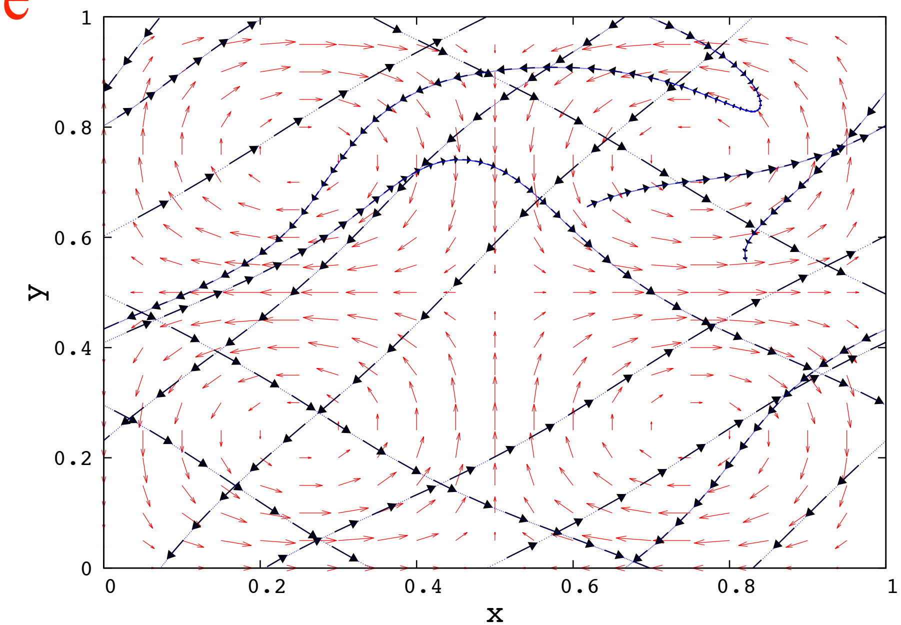
$$\dot{x} = v_x, \qquad \dot{y} = v_y$$

$$\dot{v}_x = -\frac{1}{\tau}(v_x - U_x) + F + \sqrt{2D_0}\xi_x$$

$$\dot{v}_y = -\frac{1}{\tau}(v_y - U_y) + \sqrt{2D_0}\xi_y$$

$$U_x = \frac{\partial \psi(x,y)}{\partial y}, \qquad U_y = -\frac{\partial \psi(x,y)}{\partial x}$$

Divergenceless velocity field

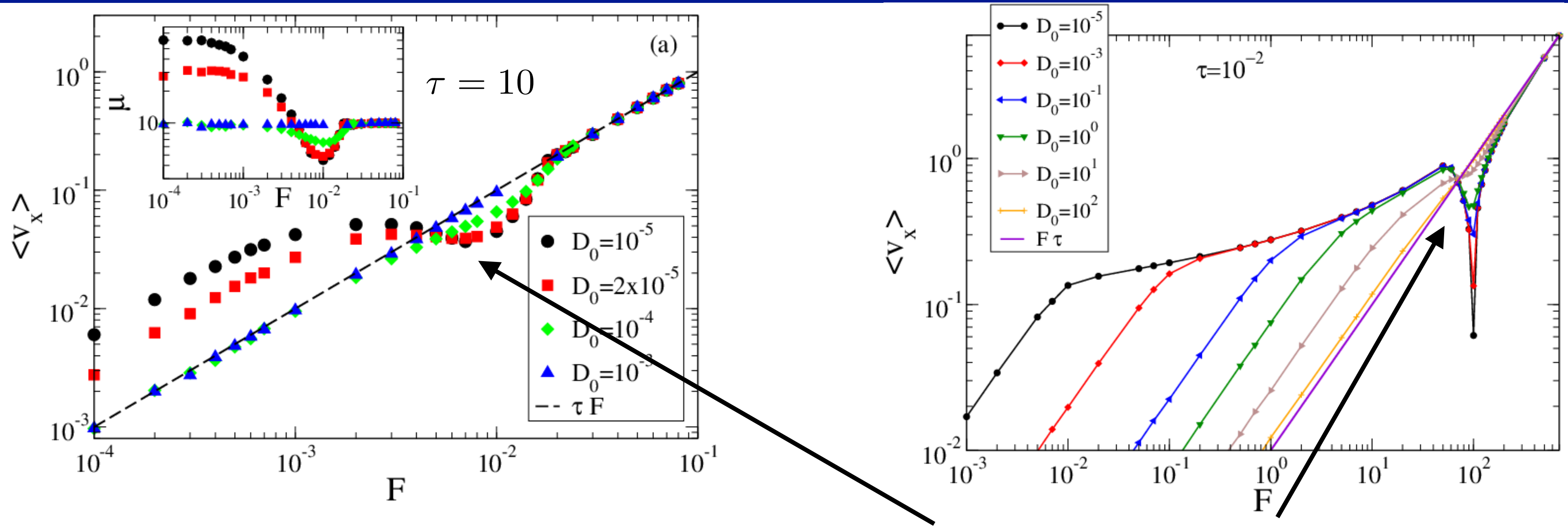


Stream function $\psi(x,y) = \frac{LU_0}{2\pi} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right)$ Stokes time τ

Parameters: $U_0 = 1,\ L = 1,\ \tau^* = L/U_0 = 1$ Characteristic time of the field

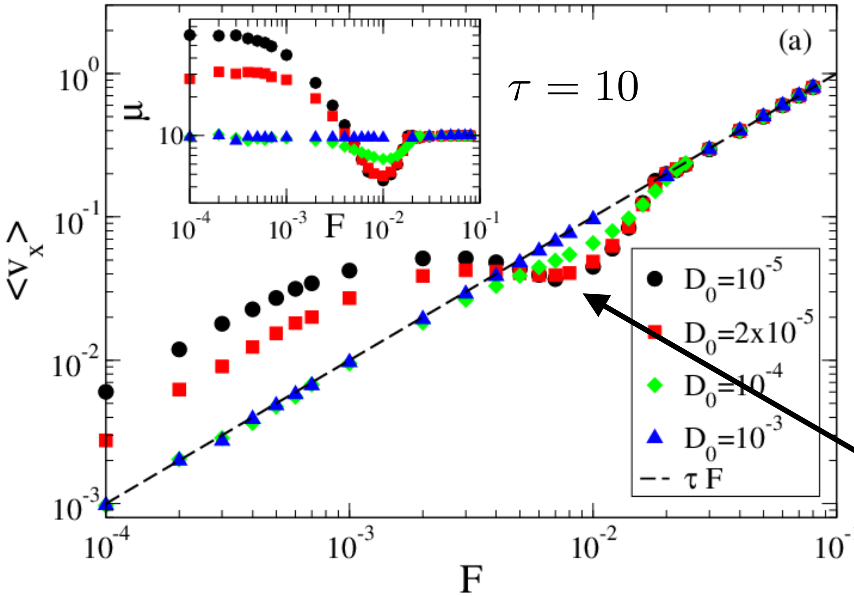
Stationary velocity $\langle v_x \rangle = F\tau + \langle U_x(x,y) \rangle$

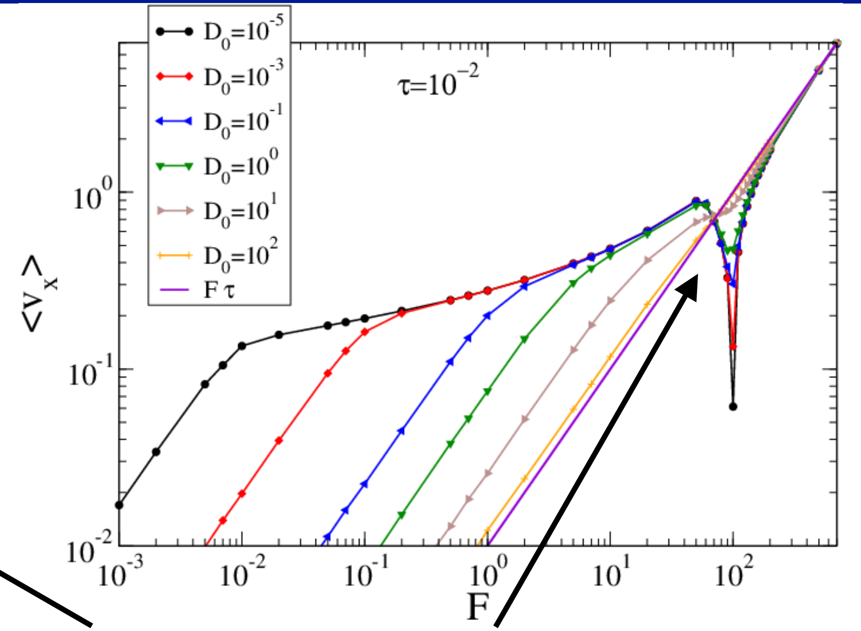
Force-velocity relation



Negative differential mobility

Force-velocity relation





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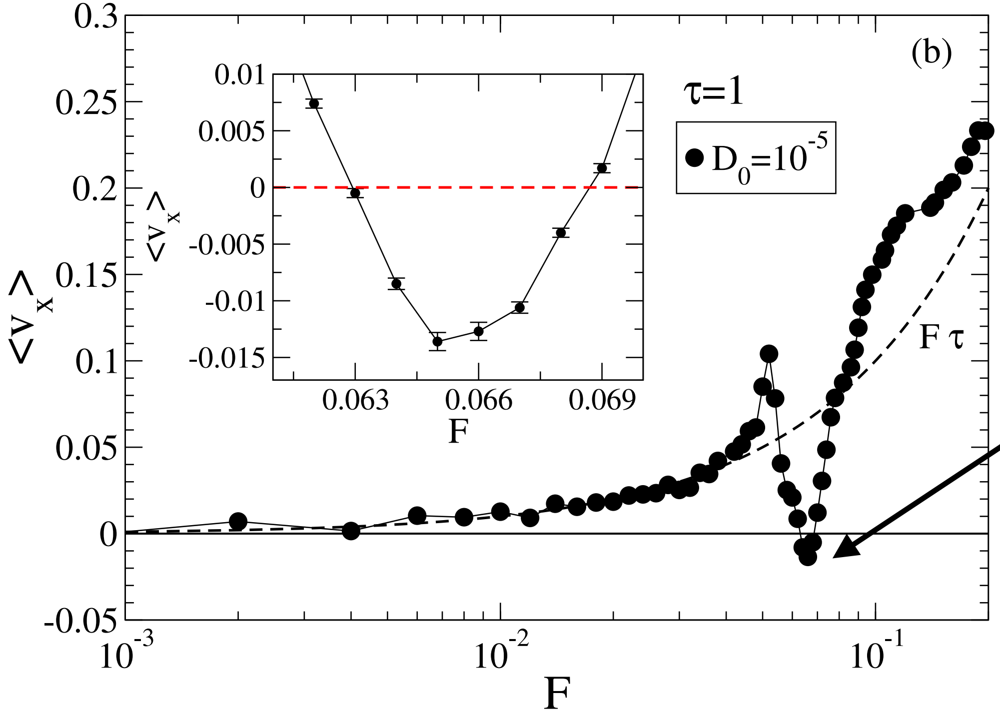
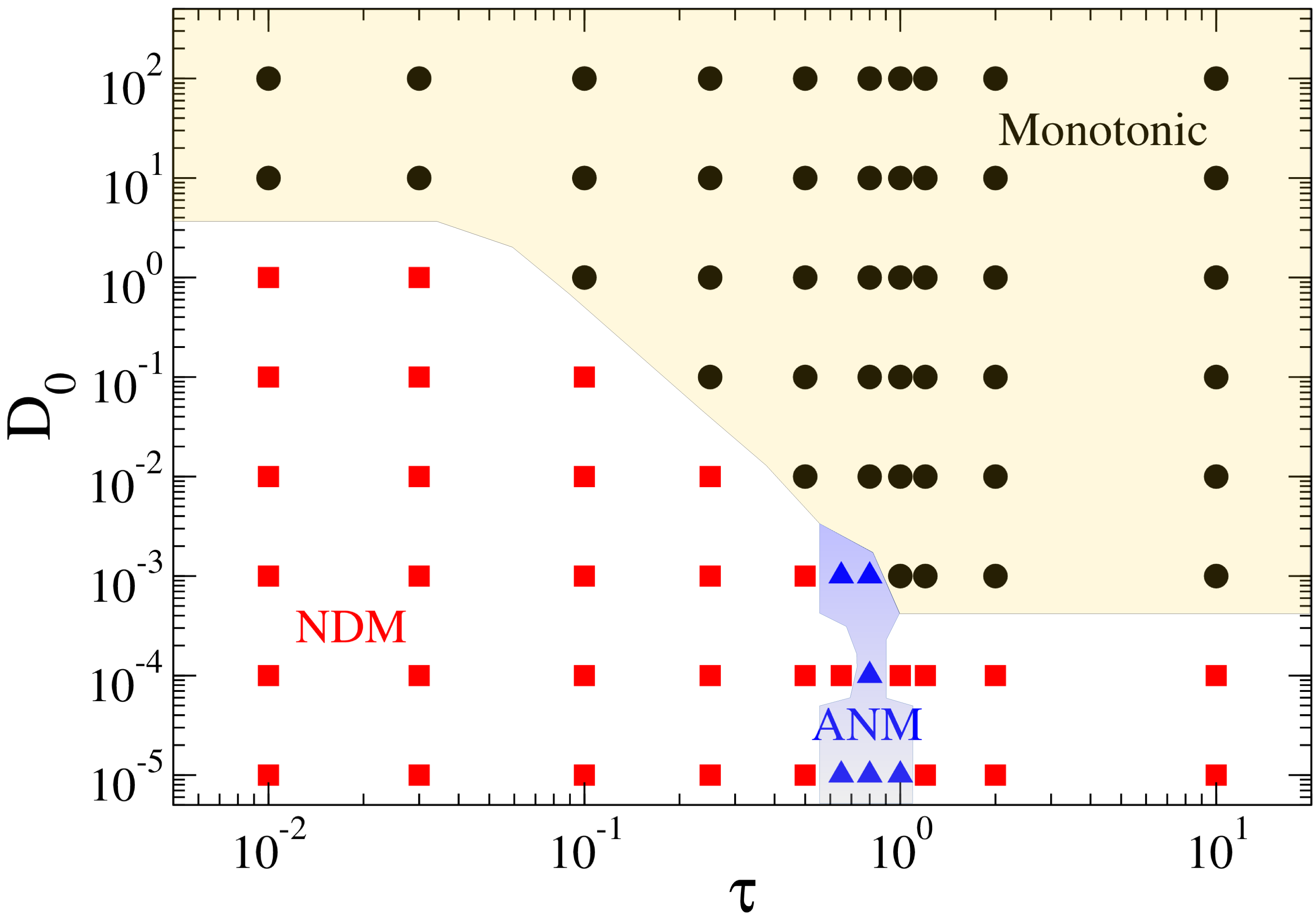


Absolute negative mobility!

for $\tau \sim \tau^* = 1$

Trapping by the underlying field

“Phase diagram”



Conclusions

Nonlinear response of a driven tracer can reveal anomalous behaviors

- Lattice gas model
  - Analytical approach
  - Negative differential mobility
  - Enhanced diffusivity induced by crowding

- Inertial particles in steady laminar flows
  - Absolute negative mobitliy

References

Microscopic theory for negative differential mobility in crowded environments
Bénichou, Illien, Oshanin, AS, Voituriez,
Phys. Rev. Lett. **113**, 268002 (2014)

Nonlinear response and emerging nonequilibrium microstructures in confined crowded environments
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Bénichou, Illien, Oshanin, AS, Voituriez,
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Tracer diffusion in crowded narrow channels.
Bénichou, Illien, Oshanin, AS, Voituriez,
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Nonlinear response of inertial tracers in steady laminar flows
AS, Cecconi, Puglisi, Vulpiani,
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Anomalous force-velocity relation of driven inertial tracers in steady laminar flows
Cecconi, Puglisi, AS, Vulpiani,
Eur. Phys. J. E **40**, 81 (2017)

Anomalous mobility of a driven active particle in a steady laminar flow
Cecconi, Puglisi, AS, Vulpiani,
J. Phys.: Condens. Matter **30**, 264002 (2018)

Thank you for your attention!

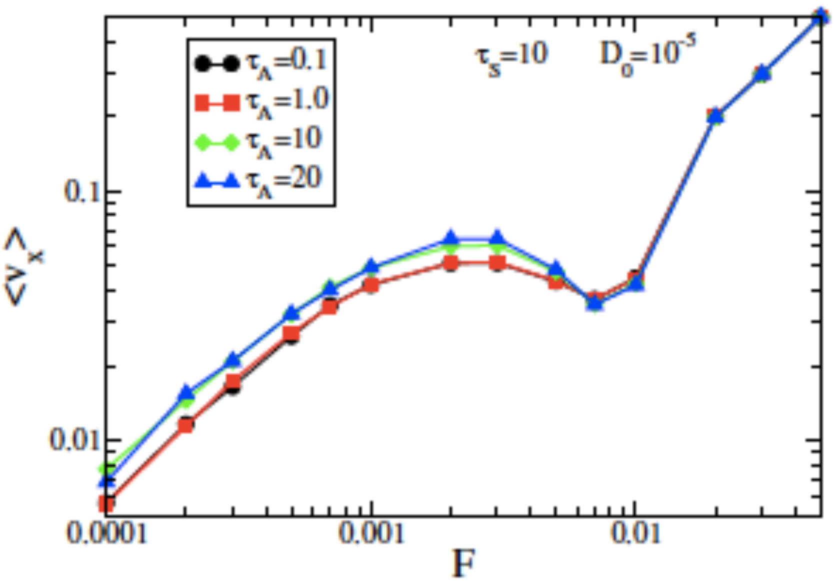
Active Ornstein Uhlenbeck Particle

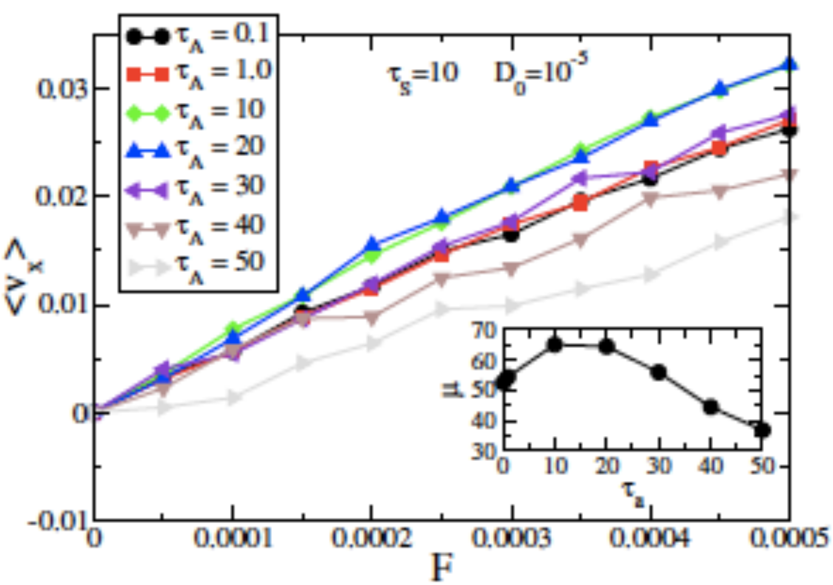
Colored noise with persistence time τ_A

$$\dot{w}_x = \frac{w_x}{\tau_A} + \frac{\sqrt{2D_0}}{\tau_A}\xi_x \qquad \dot{w}_y = \frac{w_y}{\tau_A} + \frac{\sqrt{2D_0}}{\tau_A}\xi_y$$

$\tau_A \to 0$ Uncorrelated noise

$\tau_A \to \infty$ Deterministic (zero-noise) dynamics





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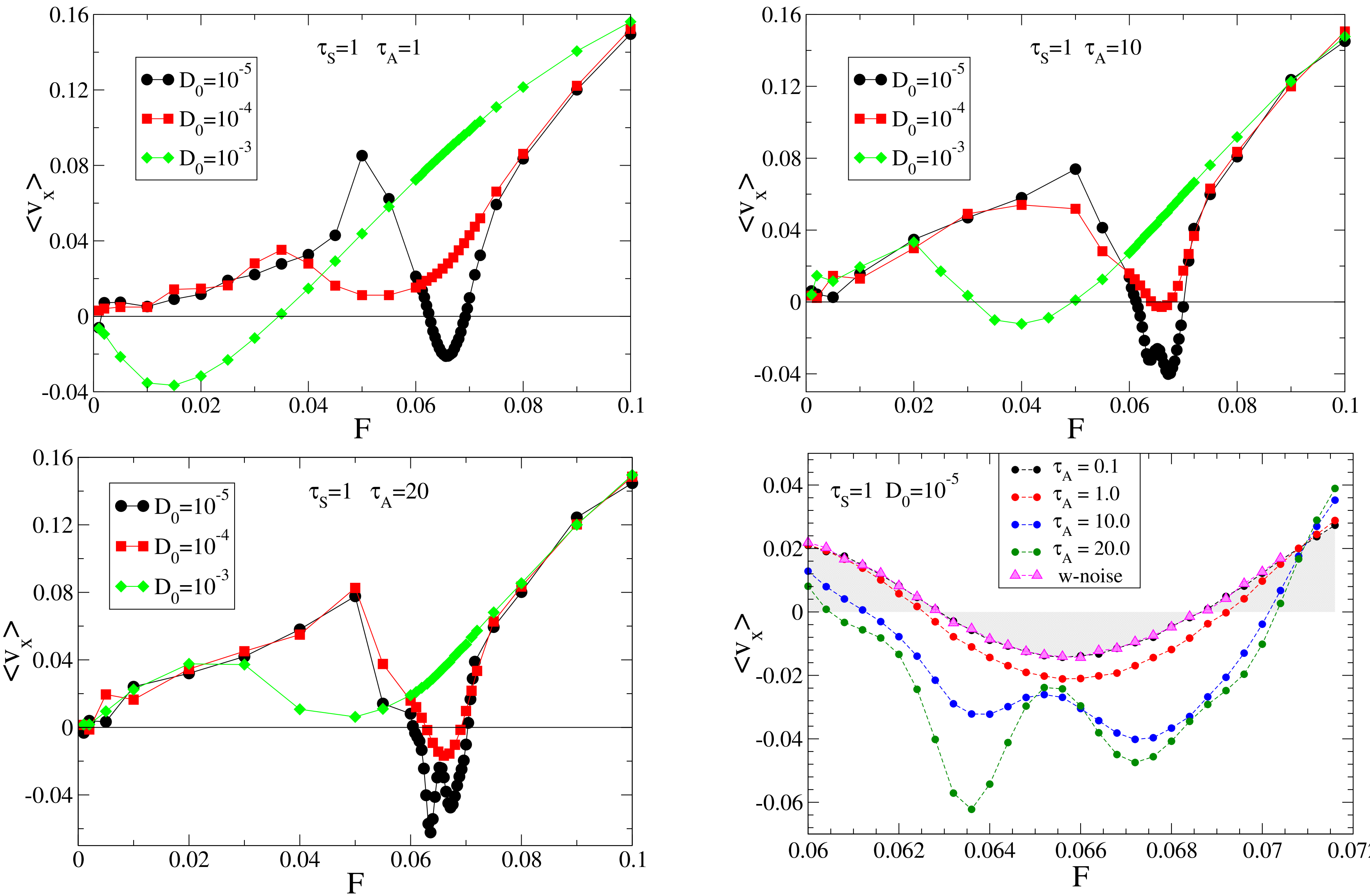
Absolute negative mobility



Argument for NDM at low density

Strong external force $\epsilon = 2e^{-\beta F/2} \ll 1$

$$p_1 = 1 - \epsilon \qquad p_{-1} = O(\epsilon^2) \qquad p_{\mu \neq \pm 1} = \frac{\epsilon}{2d - 2}$$

Force-velocity relation: $$V(F) = \frac{\text{mean distance}}{\text{mean time of free flight} + \text{mean trapping time}}$$

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Mean distance between two obstacles $1/\rho$

Mean duration of free flight $\tau/[\rho(1-\epsilon)]$

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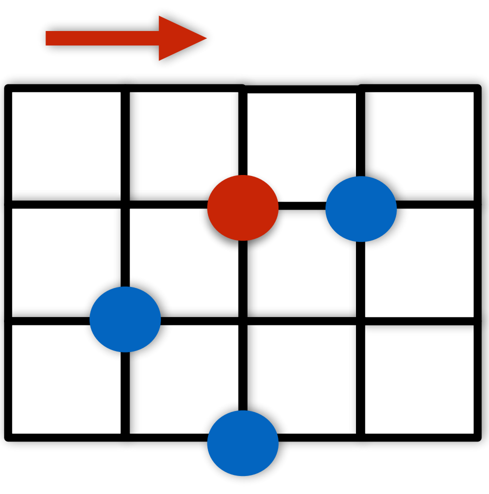
tracer steps in a transverse direction



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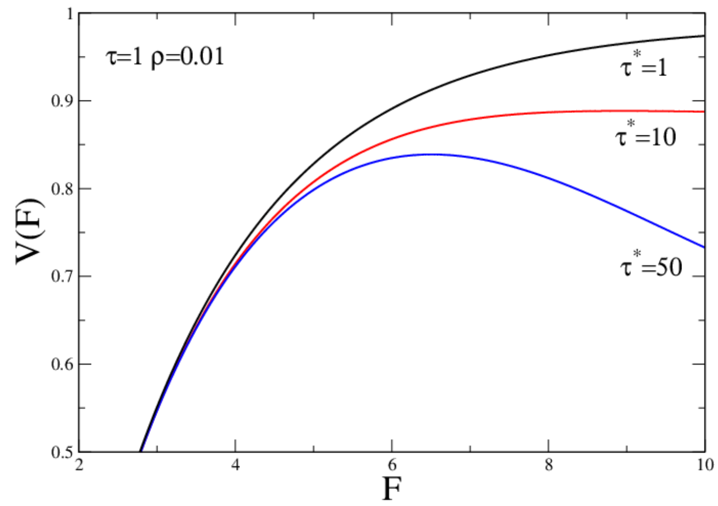
$$V(F) = \frac{1-\epsilon}{\tau + 4\rho(1-\epsilon)\frac{\tau^*}{3+4\epsilon\tau^*/\tau}}$$

Criterion for NDM $\tau^*/\tau \gtrsim \rho^{-1/2}$



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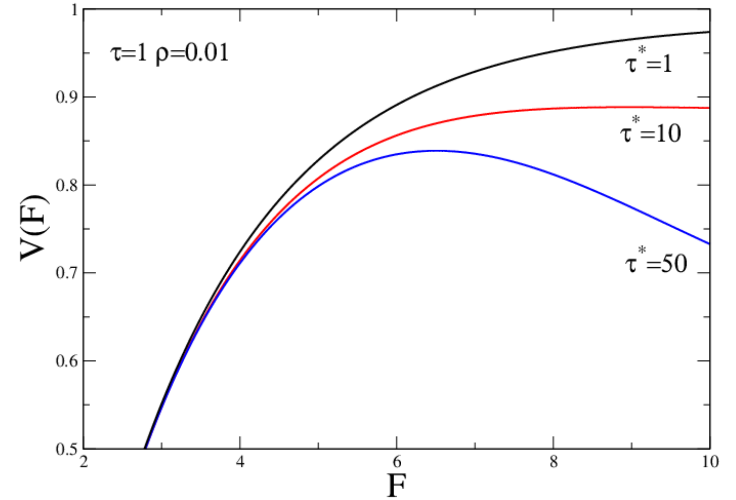

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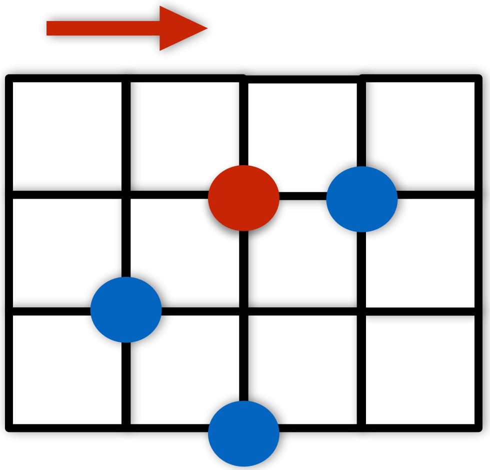

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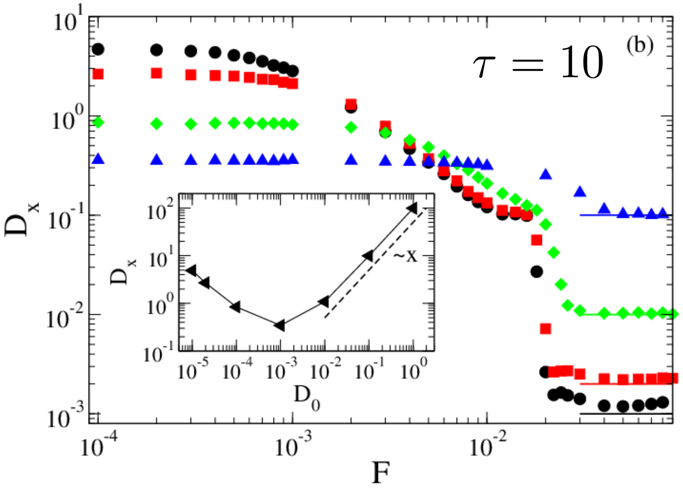
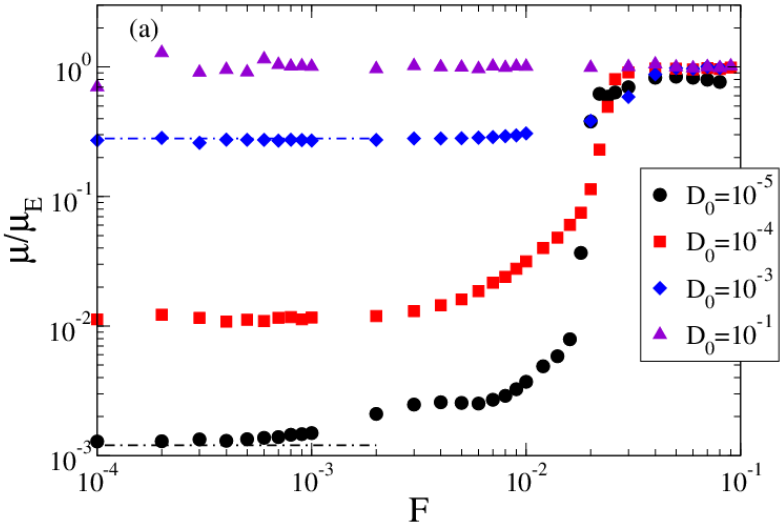
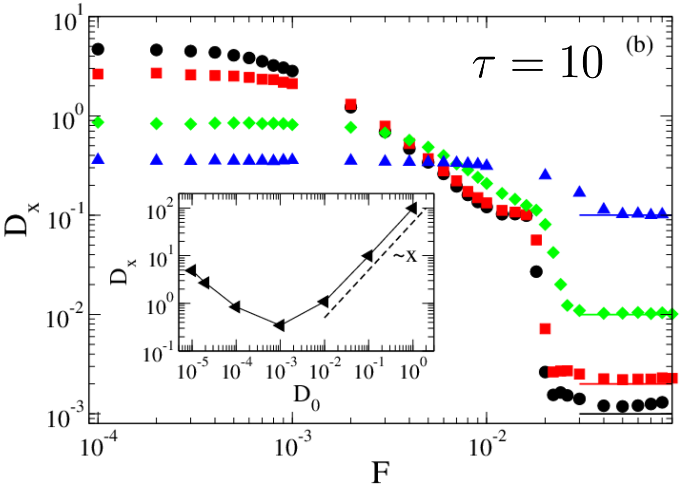
Generalized Einstein relation

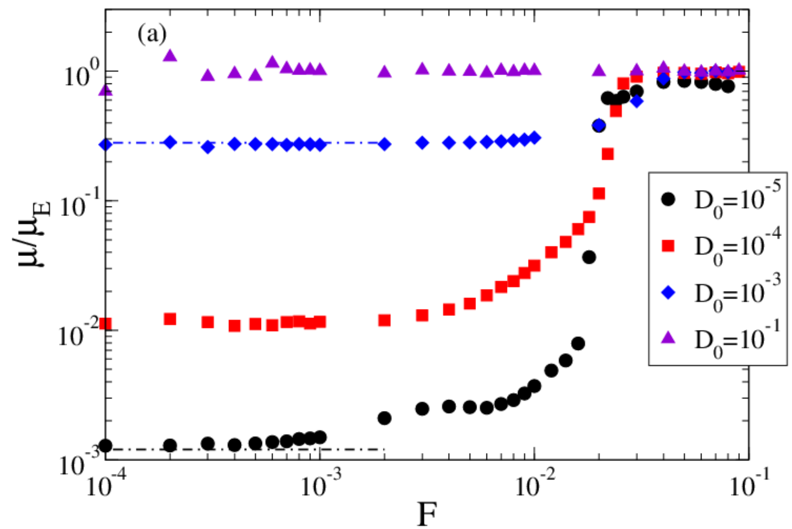




Einstein relation $\mu = \mu_E \equiv \frac{1}{T} D_x$

Generalized Einstein relation





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Baiesi, Maes, Wynants J.Stat.Phys. (2010)

Nonequilibrium extra-term

$$\mu_0 = \frac{1}{T}[D_x(F=0) - C_{x\Phi}(F=0)]$$

$$C_{x\Phi}(F) = \lim_{t\to\infty} \frac{1}{2Tt}\langle [x(t) - x(0)]\Phi(t)\rangle_{c,F}$$

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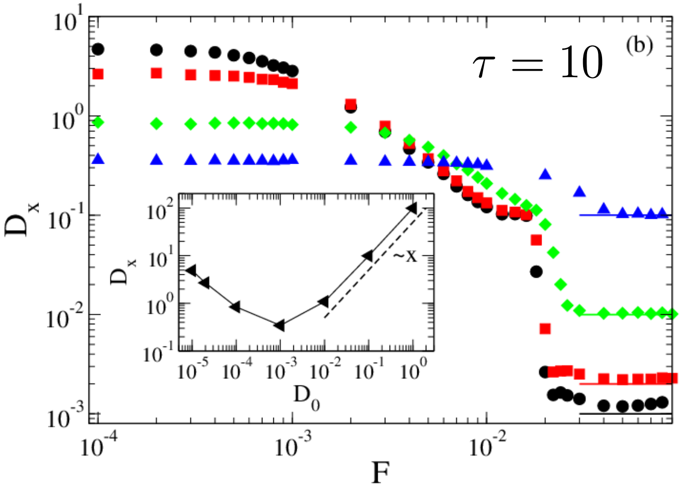

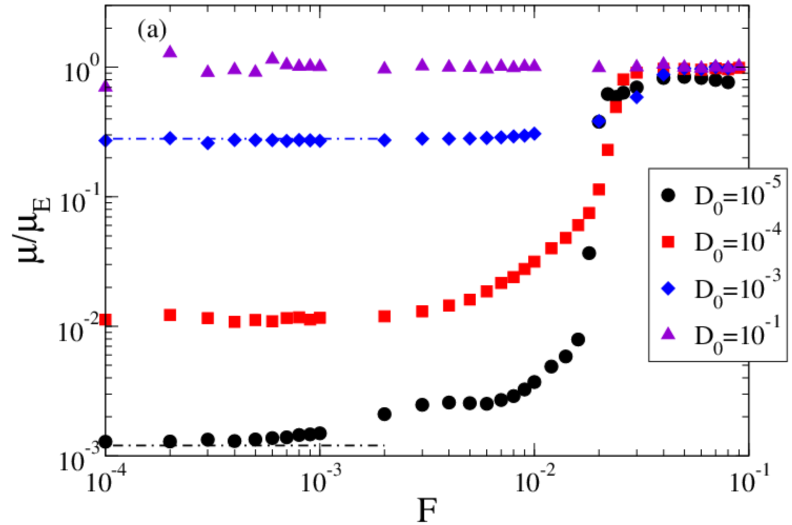

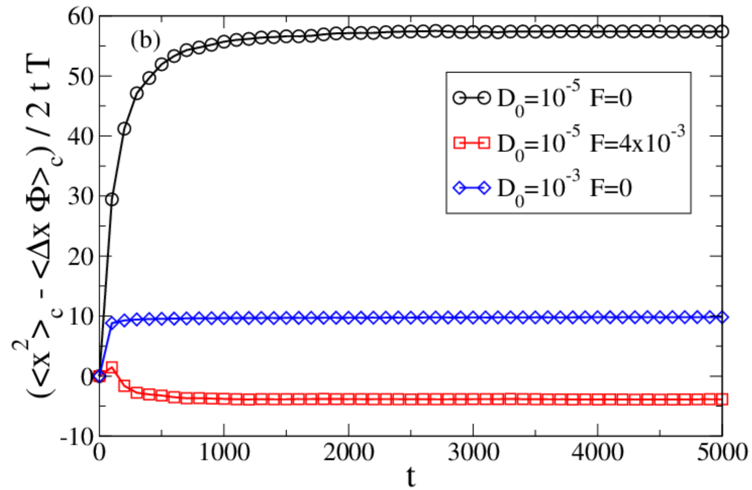

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NDM and ANM interpreted as the consequence of $C_{x\Phi} > D_x$

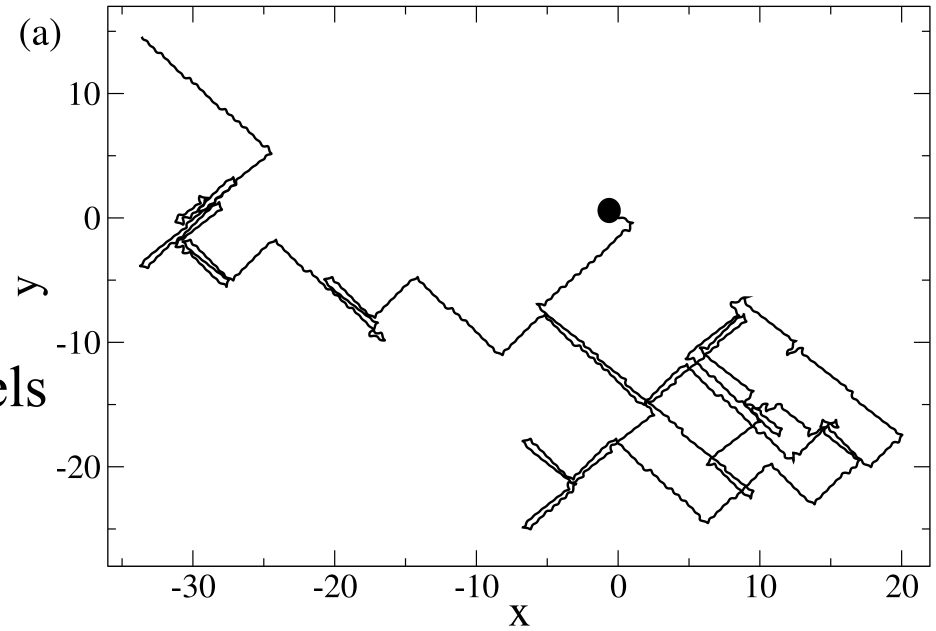
Basu & Maes J. Phys. A (2014)

Possible physical mechanism

Typical trajectory for $D_0 = 0$

The motion is realized along preferential "channels"

Both inertia and noise activate random transitions between the channels



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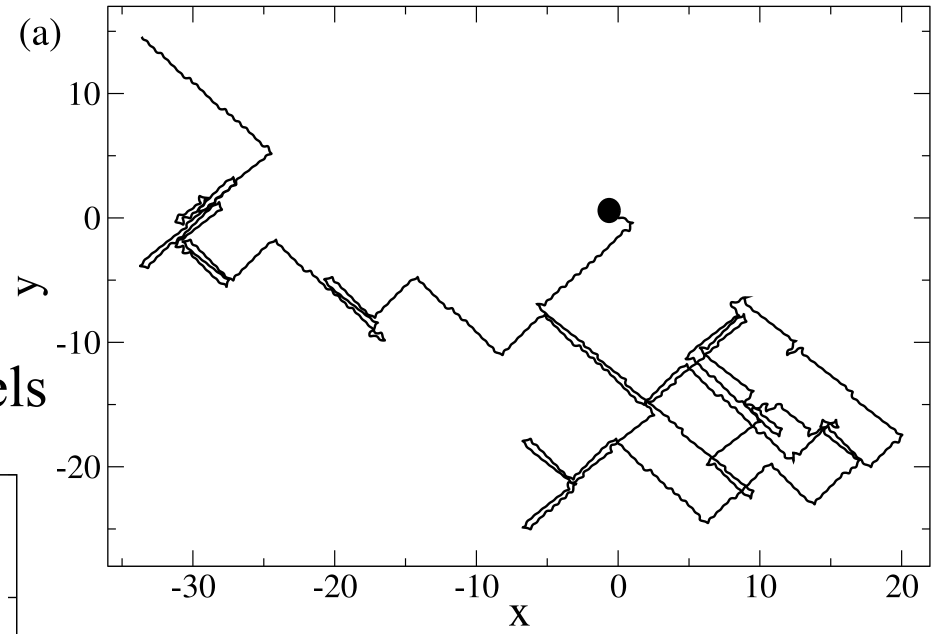

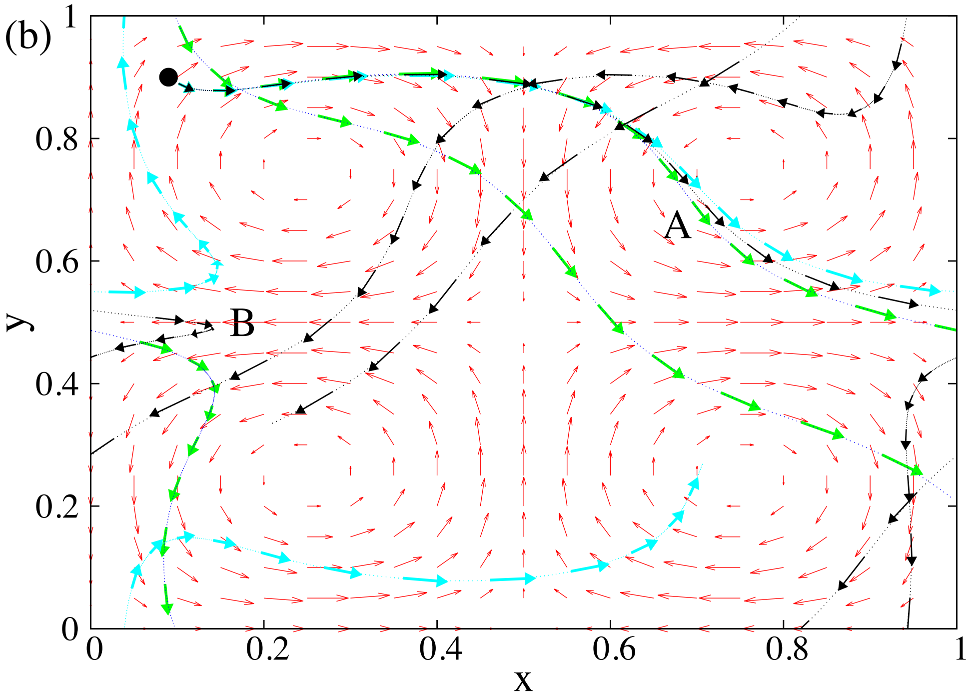

F=0.065

The tracer is pushed from region A (downstream channel) to region B (upstream channel)

F=0.04

F=0.09

With a smaller or larger force, the particle avoids the adverse region B and continues its run along downstream channels

Decoupling approximation and analytic solution

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$$A_\nu \equiv 1 + \frac{2d\tau^*}{\tau} p_\nu (1 - k(\boldsymbol{e}_\nu))$$

Density profile
around the tracer

$$k(\lambda; t) = \sum_{\boldsymbol{R}_{TP}, \eta} \eta(\boldsymbol{R}_{TP} + \lambda) P(\boldsymbol{R}_{TP}, \eta; t)$$

occupation variable

Decoupling approximation and analytic solution

Master Equation for $P(\boldsymbol{R}_{TP}, \eta; t)$

$\boldsymbol{R}_{TP}$ tracer position

η obstacle configuration

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occupation variable

$$2d\tau^* \partial_t k(\lambda; t) = \sum_\mu \left(\nabla_\mu - \delta_{\lambda, \mathbf{e}_\mu} \nabla_{-\mu}\right) k(\lambda; t) + \frac{2d\tau^*}{\tau} \sum_\nu p_\nu \langle [1 - \eta(\boldsymbol{R}_{TP} + \mathbf{e}_\nu)] \nabla_\nu \eta(\boldsymbol{R}_{TP} + \lambda) \rangle$$

Transition rates out of equilibrium

Decoupling approximation ➡ General solution

Tracer velocity $$V(F) \equiv \frac{d\langle \boldsymbol{R}_{TP} \cdot \boldsymbol{e}_1 \rangle}{dt} = \frac{1}{2d\tau^*}(A_1 - A_{-1})$$

$$A_\nu = 1 + \frac{2d\tau^*}{\tau} p_\nu \left[1 - \rho - \rho(A_1 - A_{-1}) \frac{\det C_\nu}{\det C} \right]$$

Significant dependence on the choice of transition probabilities?

Transition rates out of equilibrium

General form of transition rates $k(\boldsymbol{x},\boldsymbol{y}) = \psi(\boldsymbol{x},\boldsymbol{y}) e^{S(\boldsymbol{x},\boldsymbol{y})/2} \delta(K.C.)$

→ $\psi(\boldsymbol{x},\boldsymbol{y}) = \psi(\boldsymbol{y},\boldsymbol{x}) \geq 0$ Symmetric (kinetic) part

→ $S(\boldsymbol{x},\boldsymbol{y}) = -S(\boldsymbol{y},\boldsymbol{x})$ Antisymmetric part

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Local detailed balance imposes a constraint on the antisymmetric part

$S(\boldsymbol{x},\boldsymbol{y}) \propto \text{entropy flux}$ ⇒ $S(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_\nu) = \beta \boldsymbol{F} \cdot \boldsymbol{e}_\nu$

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Arbitrary choice for the symmetric part

Leitmann & Franosch, Bénichou et al. $\psi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_\nu) = 1/\tau[e^{\beta F/2} + e^{-\beta F/2} + 2]$

Basu & Maes
$$\begin{cases} \psi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_\nu) = 1/2\tau[e^{\beta F/2} + e^{-\beta F/2}] \;\; \text{for} \;\; \nu = \pm 1 \\ \psi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_\nu) = 1/4\tau \;\; \text{for} \;\; \nu = \pm 2 \end{cases}$$

independent of F in the transverse direction

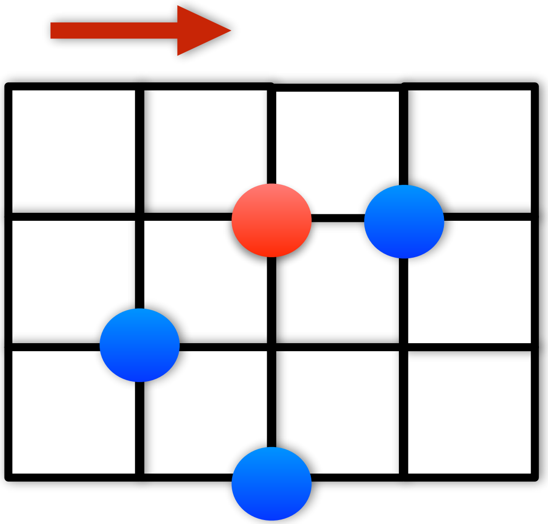
Role of the transition probabilities

$$p_\nu = \frac{e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\nu}}{\sum_\mu e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\mu}}$$

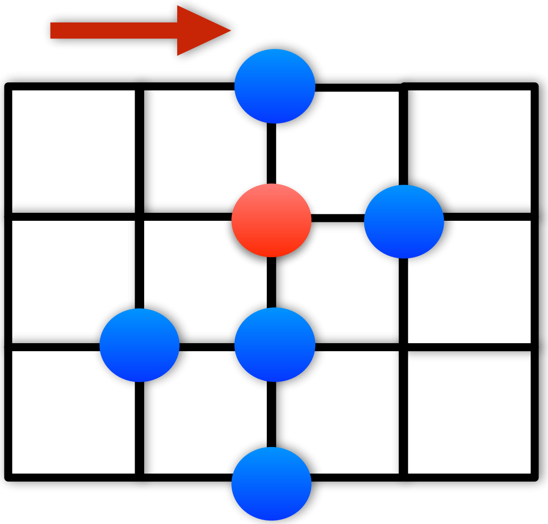
(Leitmann & Franosch, Bénichou et al.)

$$p_\uparrow = p_\downarrow = \frac{1}{4}$$ independent of F

(Basu & Maes)



One obstacle can create a long lived trap



No trapping effect at linear order in the density

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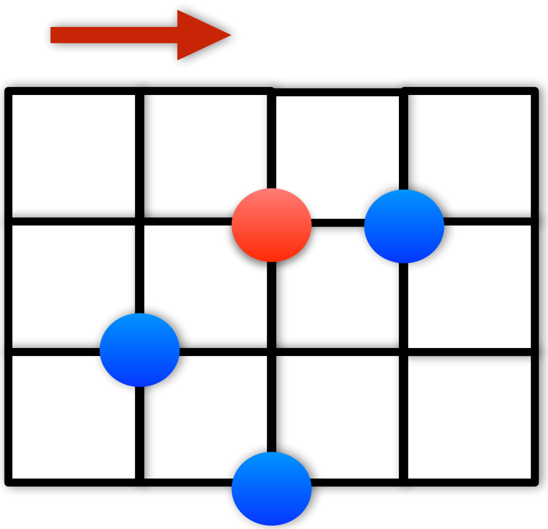

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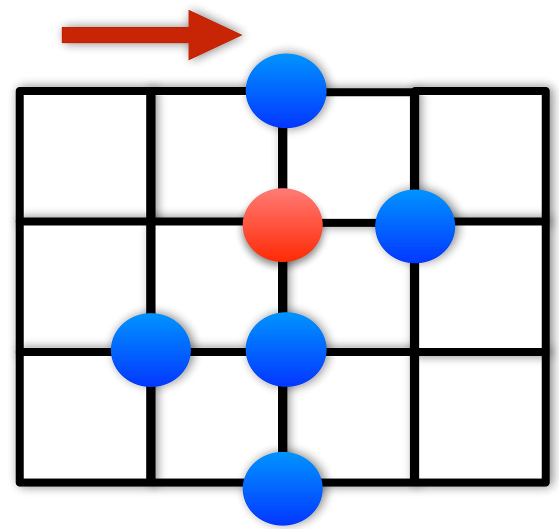


No trapping effect at linear order in the density

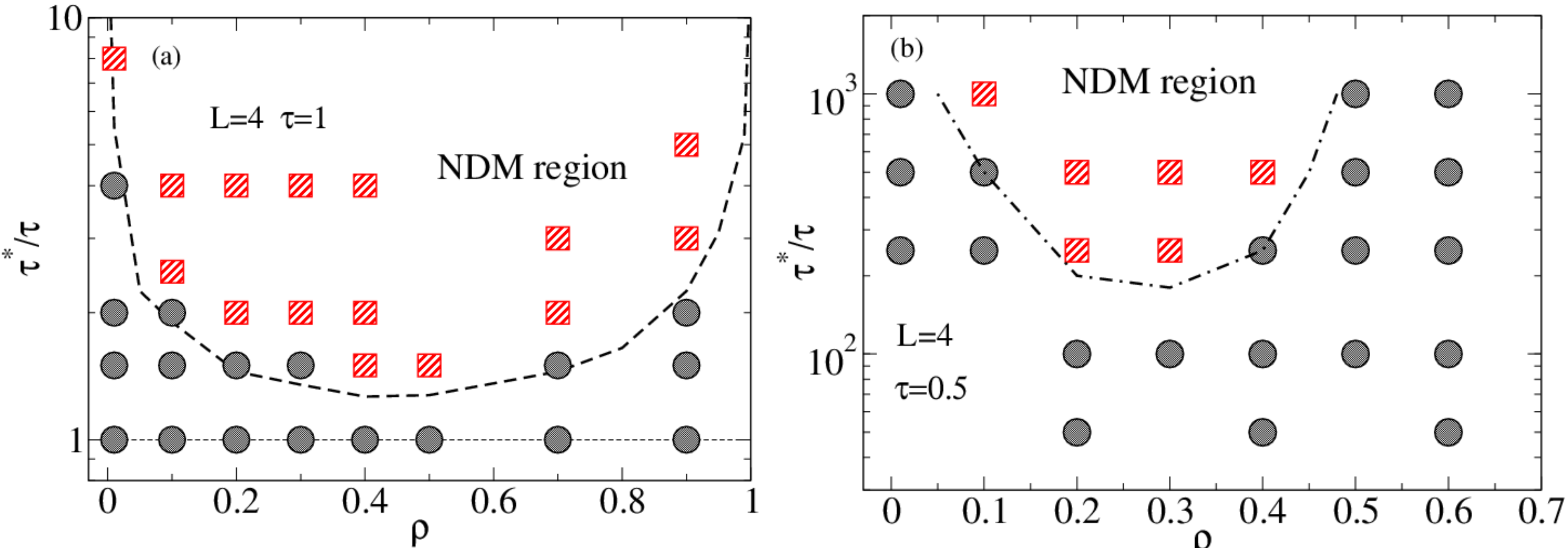
Different choices → significant macroscopic differences

(Baiesi et al. PRE (2015))

Warning: how to define microscopic transition rates out of equilibrium?

Criterion for negative differential mobility

Parameter space: time scales τ^*/τ and density ρ



$$p_\nu = \frac{e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\nu}}{\sum_\mu e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\mu}}$$

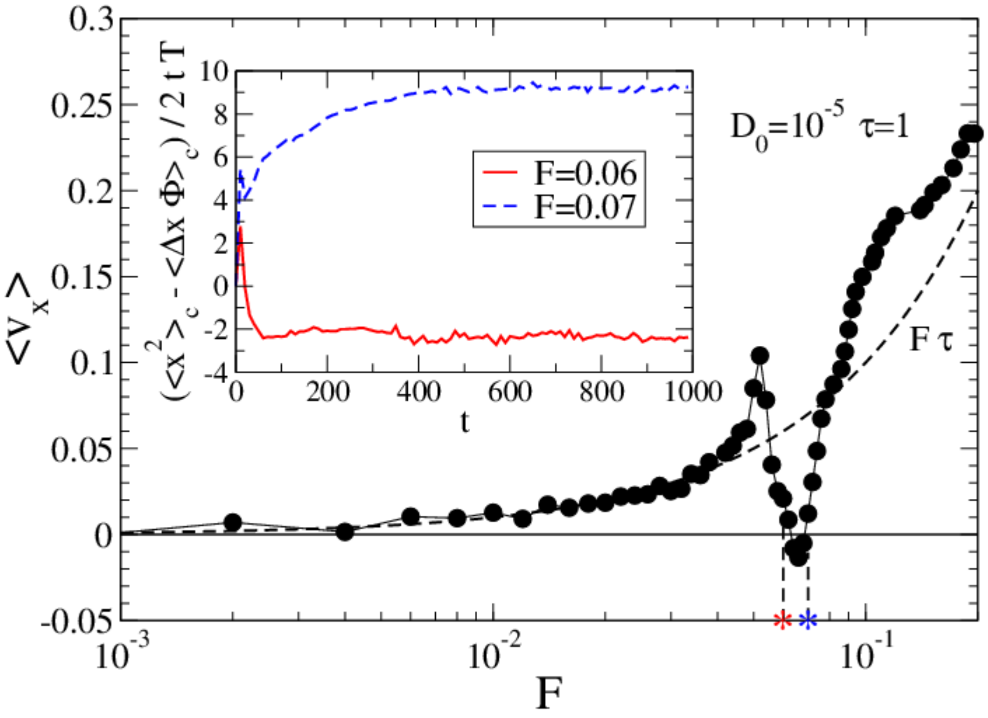
$$p_\uparrow = p_\downarrow = \frac{1}{4}$$ independent of F

NDM is robust, but the phase chart is different

Absolute negative mobility

Force-velocity relation for

$$\tau = 1$$



the GER is verified, showing strong negative and positive differential mobilities just before and just after the minimum

Decoupling approximation and analytic solution

Master Equation for $P(\boldsymbol{R}_{TP}, \eta; t)$

$\boldsymbol{R}_{TP}$ tracer position

η obstacles configuration

$$\begin{aligned}
\partial_t P(\boldsymbol{R}_{TP}, \eta; t) &= \frac{1}{2d\tau^*} \sum_{\mu=1}^{d} \sum_{\boldsymbol{r} \neq \boldsymbol{R}_{TP} - \boldsymbol{e}_\mu, \boldsymbol{R}_{TP}} [P(\boldsymbol{R}_{TP}, \eta^{\boldsymbol{r},\mu}; t) - P(\boldsymbol{R}_{TP}, \eta; t)] \\
&+ \frac{1}{\tau} \sum_{\mu=1}^{d} p_\mu \{[1 - \eta(\boldsymbol{R}_{TP})] P(\boldsymbol{R}_{TP} - \boldsymbol{e}_\mu, \eta; t) \\
&- [1 - \eta(\boldsymbol{R}_{TP} + \boldsymbol{e}_\mu)] P(\boldsymbol{R}_{TP}, \eta; t)\}
\end{aligned}$$

Tracer velocity $$V(F) \equiv \frac{d\langle \boldsymbol{R}_{TP} \cdot \boldsymbol{e}_1 \rangle}{dt} = \frac{1}{2d\tau^*}(A_1 - A_{-1})$$

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Density profile $$k(\lambda; t) = \sum_{\boldsymbol{R}_{TP}, \eta} \eta(\boldsymbol{R}_{TP} + \lambda) P(\boldsymbol{R}_{TP}, \eta; t)$$

PART II: nonlinear response of an inertial tracer

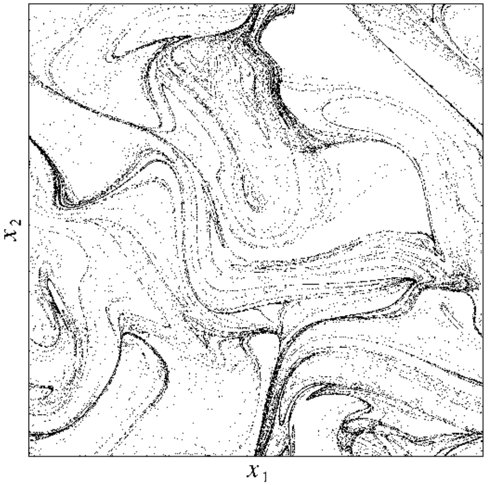
Transport properties of particles of non-negligible mass in fluids

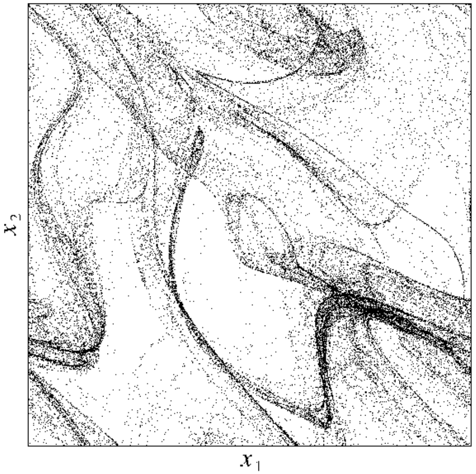
➡ Sedimentation, dispersion of pollutants, rain formation in clouds…

Inertia implies non-trivial deviations from the trajectory of fluid particles

Strongly inhomogeneous distributions

Preferential concentration





Bec (2005); De Lillo, Cecconi, Lacorata, Vulpiani (2008)

Steady cellular flow