Microscopic theory for negative differential mobility in crowded environments

Alessandro Sarracino

in collaboration with

O. Bénichou, P. Illien, G. Oshanin, R. Voituriez

Phys. Rev. Lett. 113, 268002 (2014)

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Outline of the talk

- Introduction on negative differential mobility (NDM)
- The model: driven tracer in a lattice gas (ASEP in a sea of SEPs)
  - Physical argument for NDM at low density
- General expression for the force-velocity relation
  - Analytical solution and the decoupling approximation
  - Criterion for NDM in the parameter space
- Transition rates out of equilibrium
  - NDM and fluctuation-dissipation relations
- Conclusions and perspectives

Passive and active microrheology

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

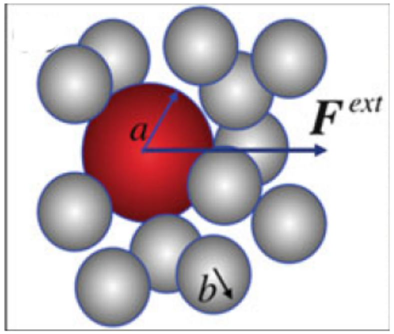
Puertas & Voigtmann (2014), Squires & Mason (2010)

Passive: probes freely diffusing in the host medium due to thermal fluctuations

Stokes-Einstein relation $D = \dfrac{k_B T}{6\pi\eta a}$

Extension to the case where the probe size is comparable to the interaction length scales relevant for the host

Active: tracer particle (TP) driven by an external force F (pulling with a constant force, or dragging at constant velocity)



Linear response connects active and passive microrheology

Extensions to the non-linear response regime $F \gg \dfrac{k_B T}{a} \approx \mathrm{pN}$

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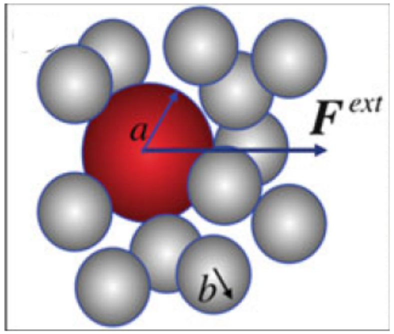

Linear response connects active and passive microrheology

Extensions to the non-linear response regime $F \gg \frac{k_B T}{a} \approx \mathrm{pN}$

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

Experimental techniques: optical and magnetic tweezers, Janus particles, etc…

Negative differential mobility

Tracer particle (TP) driven by an external force F in a host medium

The differential mobility $\mu(F) = \left.\frac{\delta V}{\delta F}\right|_{F}$ measures how the velocity increases with changing $F \to F + dF$

Negative differential mobility

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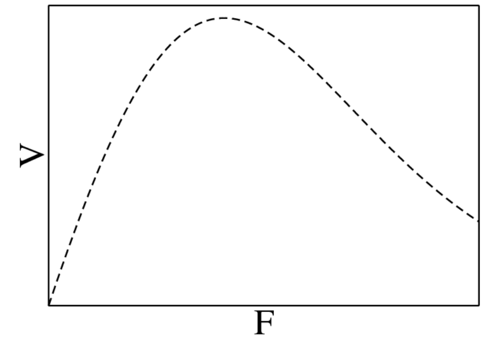
Nonlinear response regime: increasing the applied force can reduce the probe's drift velocity in the force direction $\mu(F) \leq 0$



$\Rightarrow$ $\boxed{\text{“Getting more from pushing less”}}$ (Zia et al. Am. J. Phys. 2002)

Driven tracer in a hard-core lattice gas

General many-particle interacting system, analytically tractable

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

Tracer driven by a force F
asymmetric exclusion process,
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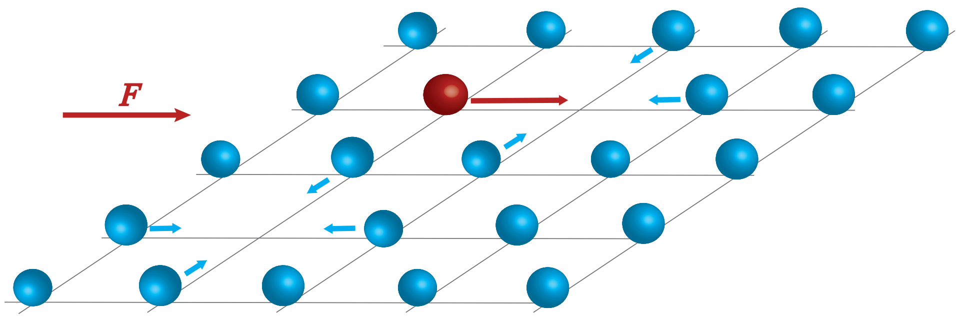

Particle density $\rho = \frac{N}{V}$

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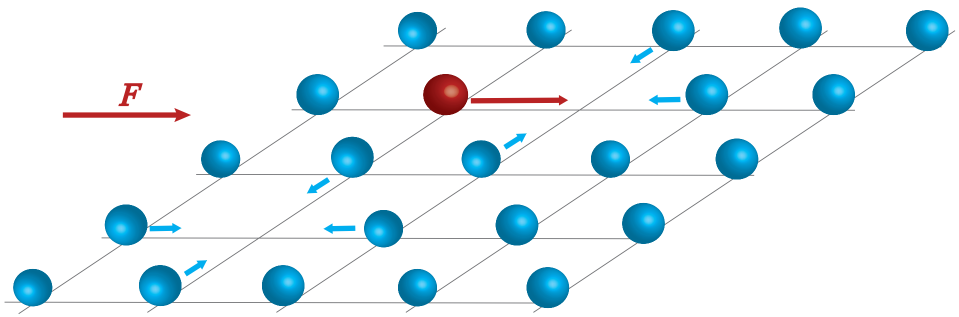

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Tracer jump probabilities

$$p_\nu = \frac{e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\nu}}{\sum_\mu e^{(\beta/2)\boldsymbol{F}\cdot\boldsymbol{e}_\mu}} \qquad \nu = \pm 1, \ldots, \pm d \quad \boldsymbol{F} = F\boldsymbol{e}_1$$

Local detailed balance $\dfrac{p_1}{p_{-1}} = e^{\beta F}$

LDB does not determine univocally the transition rates

Force-velocity relation in a hard-core lattice gas

Study of the force-velocity relation $V(F)$ and NDM phenomenon

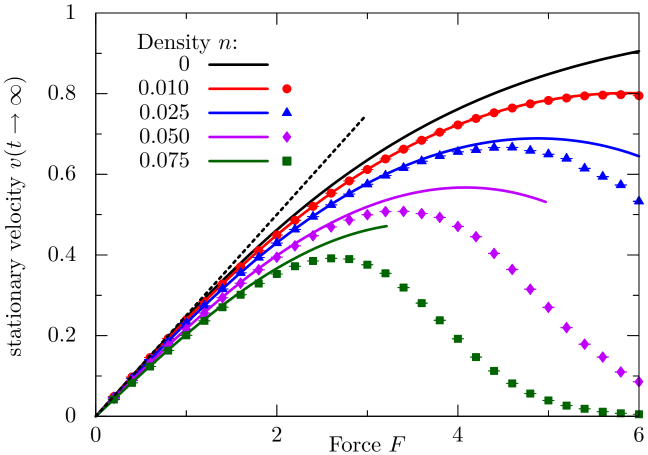
Previous results in specific cases:

Fixed obstacles (Lorentz gas)

$$\tau^*/\tau = \infty$$

analytic results at low density

Leitmann & Franosch PRL 2013

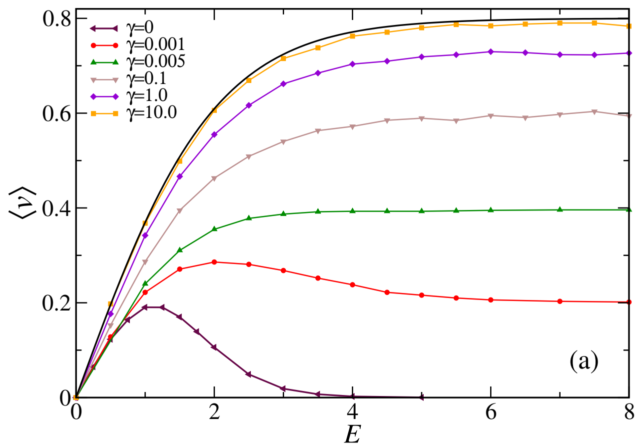


Mobile obstacles

$$\tau^*/\tau < \infty, \rho = 0.2$$

numerical analysis

Basu & Maes J. Phys. A 2014



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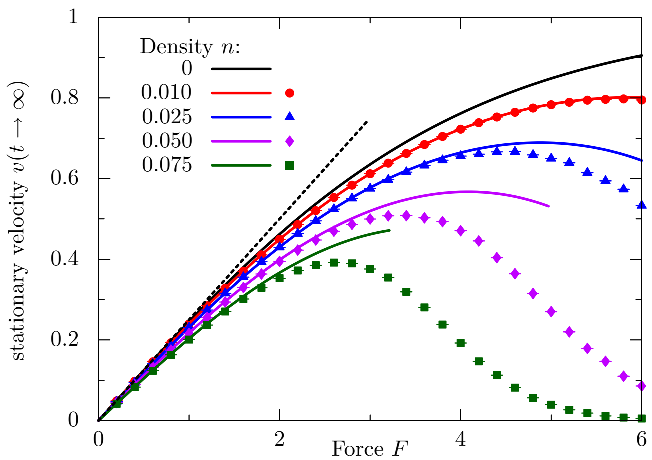

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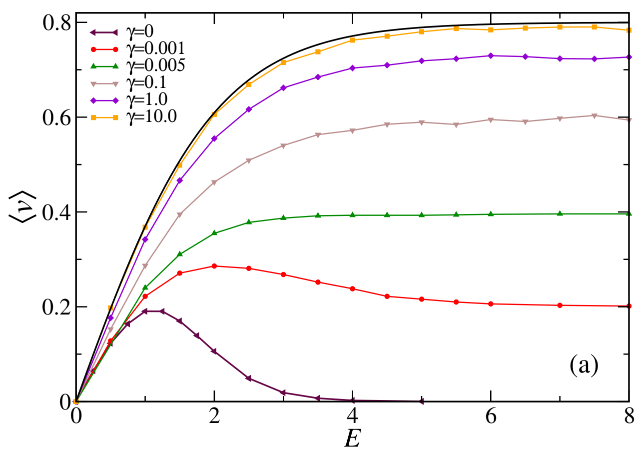

General description in all regimes?

Role of density and time scales ratio? Physical mechanism?

Argument for NDM at low density

Bénichou et al. PRL 2014

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

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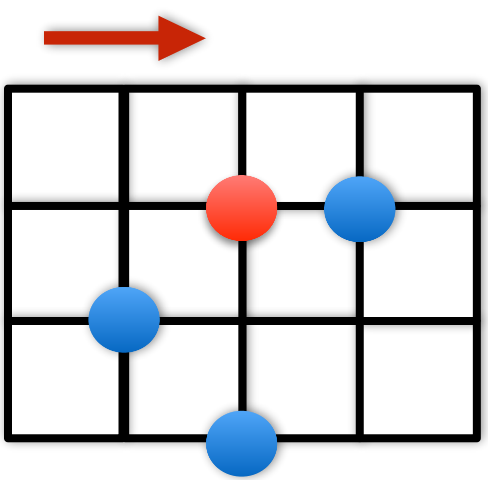
Mean distance between two obstacles $1/\rho$

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

$$1/\tau_{\mathrm{trap}} = 3/(4\tau^*) + \epsilon/\tau$$

obstacle steps away

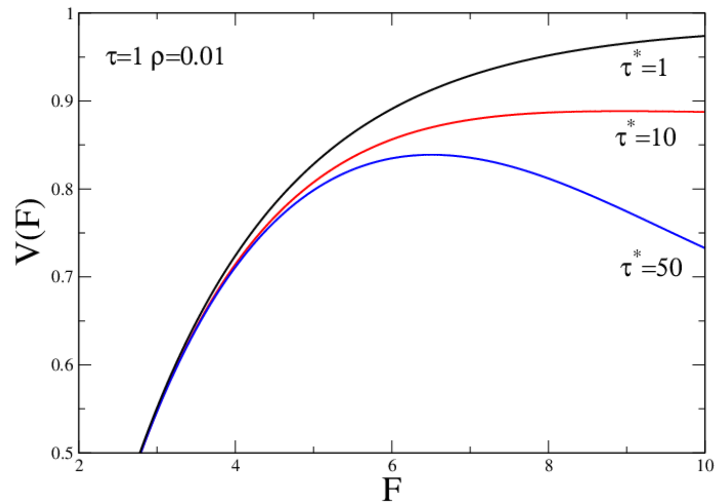
tracer steps in a transverse direction



Argument for NDM at low density

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

$$\boxed{\text{Criterion for NDM} \quad \tau^* \gtrsim \tau/\sqrt{\rho}}$$



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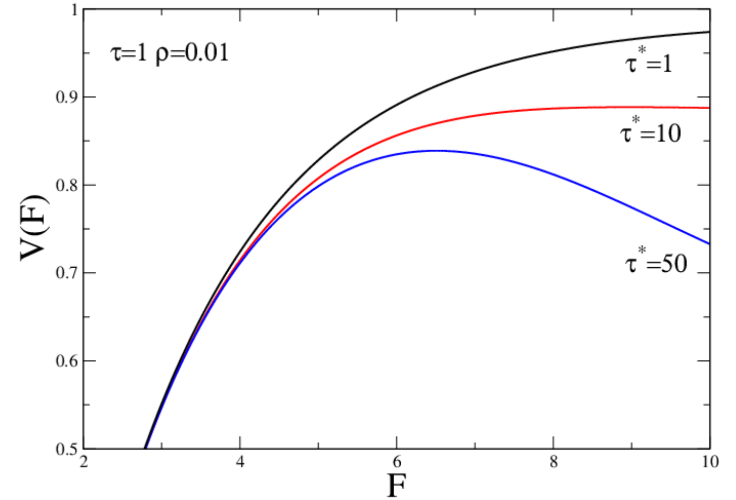

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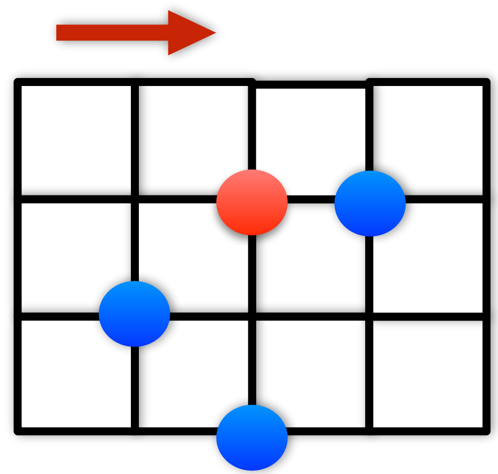
Physical mechanism: a large force

- reduces the flight time between two consecutive encounters with bath particles;
- increases the escape time from traps created by surrounding obstacles



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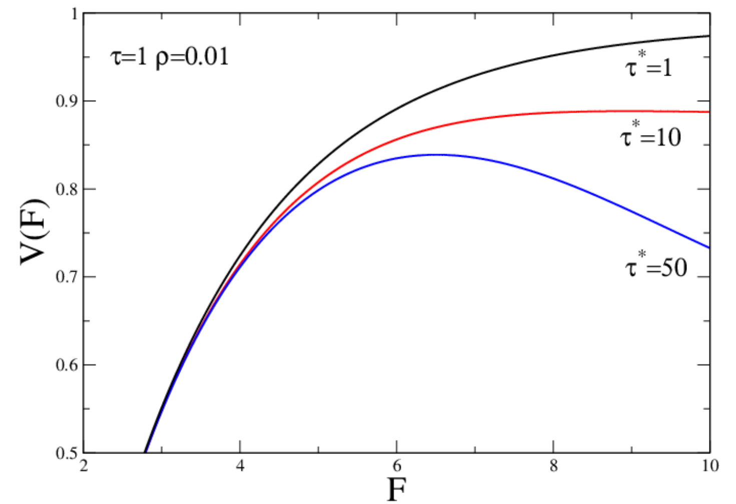

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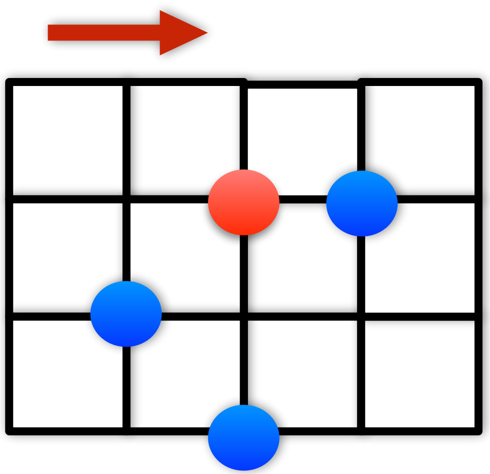

For τ^* large enough ("slow" obstacles), traps are sufficiently long lived to slow down the TP when F is increased → NDM

Master equation of the driven lattice gas

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

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

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

Decoupling approximation and analytic solution

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

Equation of motion for the density profile

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

higher order correlations are involved

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

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The decoupling approximation allows us to obtain a closed nonlinear system of equations

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

$$C \equiv (A_\mu \nabla_{-\mu} \mathcal{F}_{\boldsymbol{e}_\nu} - \alpha \delta_{\mu,\nu})_{\mu,\nu} \qquad \alpha = \sum_\mu A_\mu$$

$$C_\nu = C \to ((\nabla_1 - \nabla_{-1}) \mathcal{F}_{\boldsymbol{e}_\nu})_\nu$$

$$\mathcal{F}_{\boldsymbol{n}} = \left(\frac{A_{-1}}{A_1} \right)^{n_1/2} \int_0^\infty e^{-t} \mathrm{I}_{n_1}(2\alpha^{-1} \sqrt{A_1 A_{-1}} t) \prod_{i=2}^{d} \mathrm{I}_{n_i}(2\alpha^{-1} A_2 t) dt$$

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

Bénichou et al. PRL 2014

Linearized solution at low density

Low density limit $\rho \to 0$ Auxiliary variable $k(\boldsymbol{e}_\nu) = \rho(1 + v_{\boldsymbol{e}_\nu})$

$$V = \frac{1}{\tau}(p_1 - p_{-1}) - \frac{\rho}{\tau}(p_1 - p_{-1} + p_1 v_1 - p_{-1} v_{-1})$$

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For $\tau^* = \infty$ we recover the solution
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Leitmann & Franosch PRL 2013

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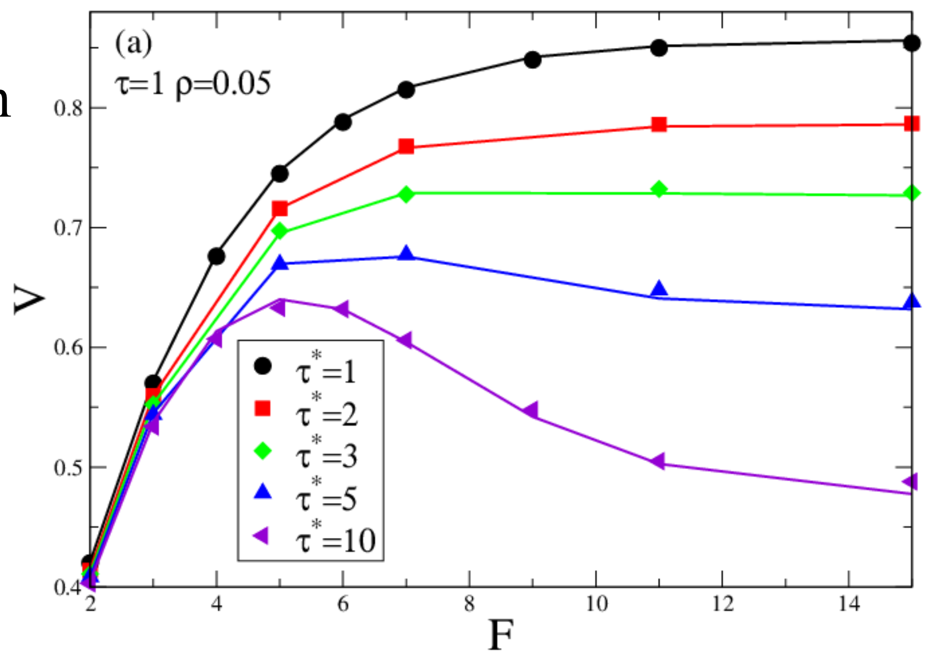
Leitmann & Franosch PRL 2013

$\boxed{\text{Exact at low density, for arbitrary } \tau^*}$



Linearized solution at low density

Explicit criterion for NDM in the parameter space

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

$$V\left(\frac{\tau^*}{\tau}\right) = V^{(0)}\left(\frac{\tau^*}{\tau}\right) + \epsilon V^{(1)}\left(\frac{\tau^*}{\tau}\right)$$

The sign of $V^{(1)}\left(\frac{\tau^*}{\tau}\right)$ determines the region of NDM

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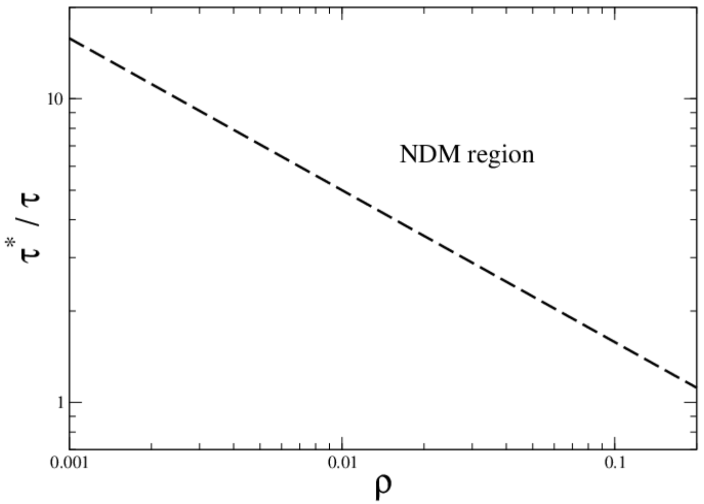
Exact asymptotic result

$$\rho \underset{\frac{\tau^*}{\tau} \to \infty}{\sim} \frac{1}{4\left(\frac{\tau^*}{\tau}\right)^2}$$



Explicit solution at high density

High density limit $\rho \to 1$ $$A_\nu = 1 + \frac{4\tau^*}{\tau} p_\nu [1 - \rho(2 + k_\nu)]$$

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Tracer velocity

$$V(\rho \to 1) = \frac{1}{\tau}(p_1 - p_{-1})(1-\rho)\frac{1}{1 + \frac{4\tau^*}{\tau}\frac{(p_1+p_{-1})(4-8/\pi)}{8/\pi}}$$

Exact result $$\boxed{V(F) = \frac{1}{\tau}(1-\rho)\frac{\sinh(\beta F/2)}{1 + \cosh(\beta F/2)[1 + \frac{2\tau^*}{\tau}(\pi - 2)]}}$$

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Bénichou & Oshanin PRE (2002)

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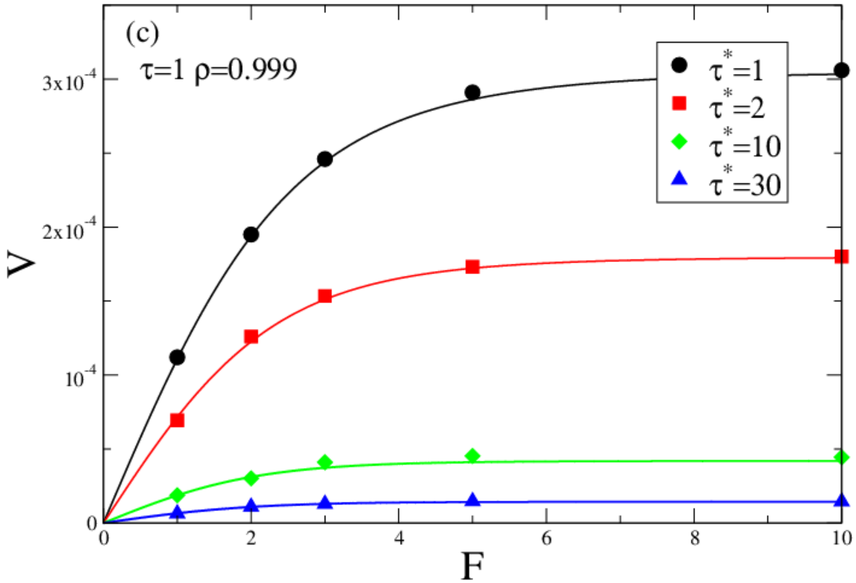
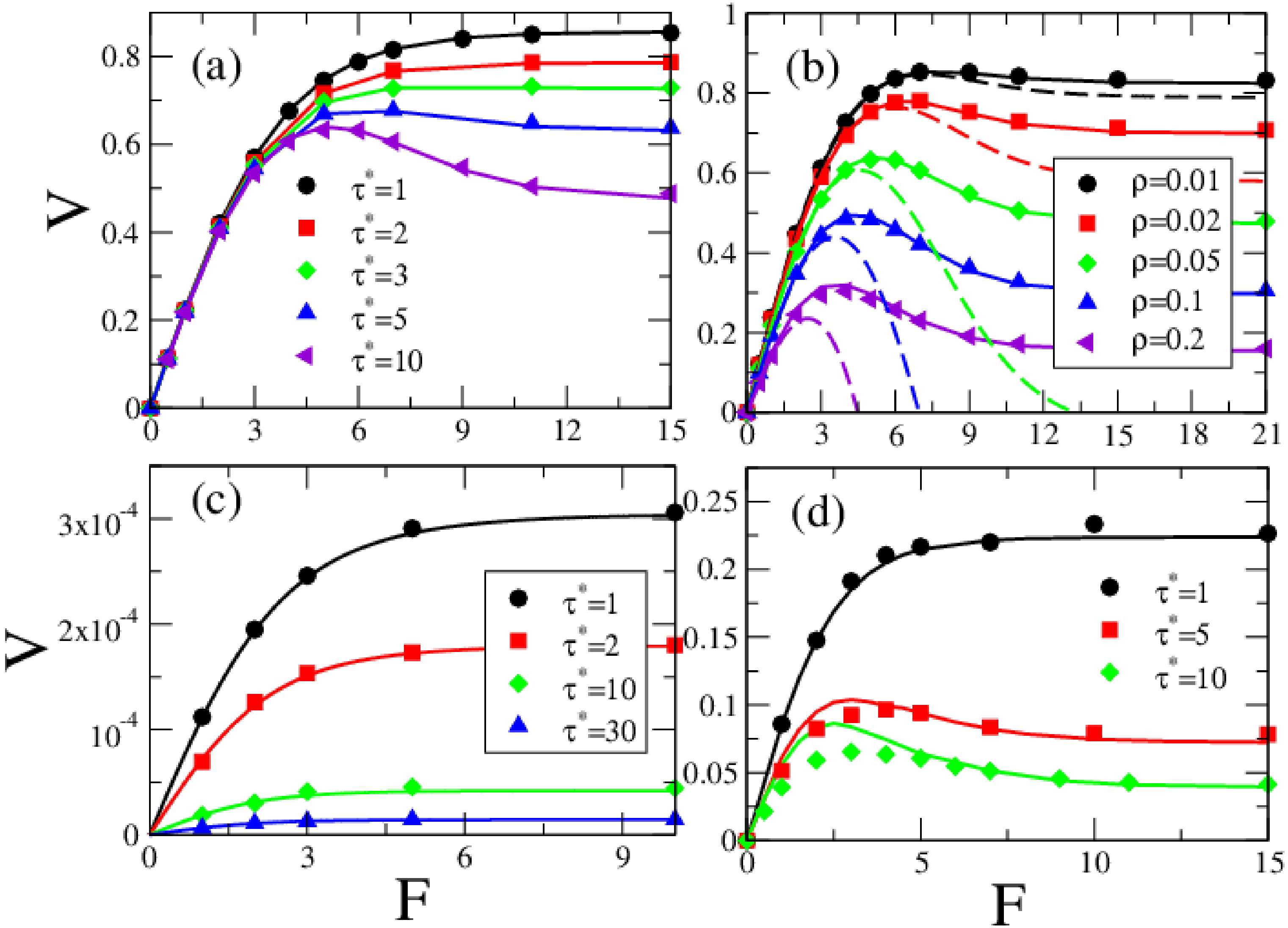


Comparison with Monte Carlo numerical simulations



$d = 2, \tau = 1$

(a) $\rho = 0.05$

(b) $\tau^* = 10$

(c) $\rho = 0.999$

(d) $\rho = 0.5$

Very good agreement in a wide range of parameters

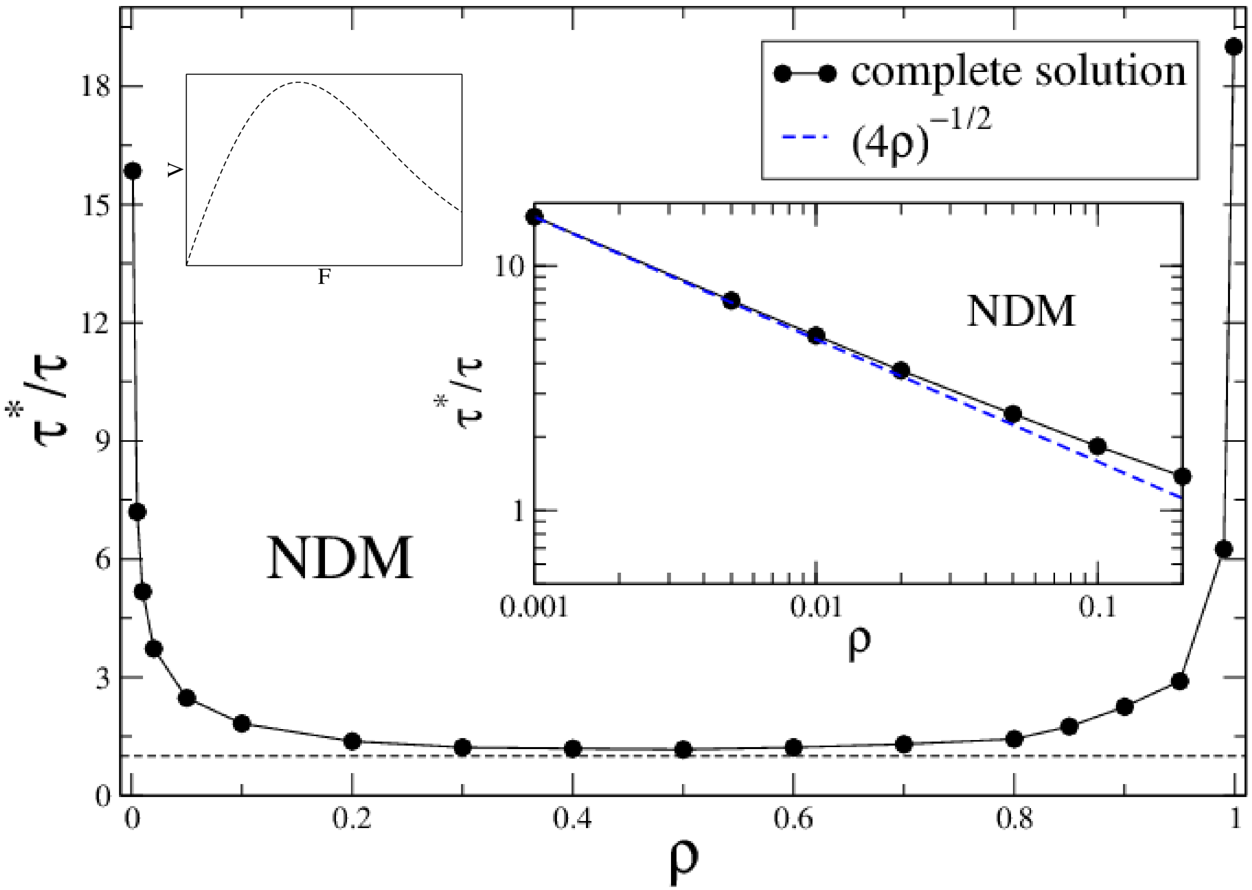
Criterion for negative differential mobility

➡ The analytical solution allows us to obtain a complete description

Phase chart in the parameter space:

time scales τ^* / τ

and density ρ



Physical mechanism: coupling between density and time scales ratio

Transition rates out of equilibrium

Decoupling approximation → General solution

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

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

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

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

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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

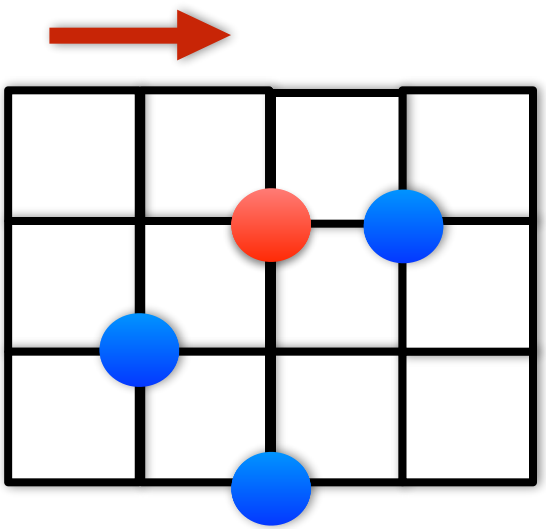
Role of the transition probabilities

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

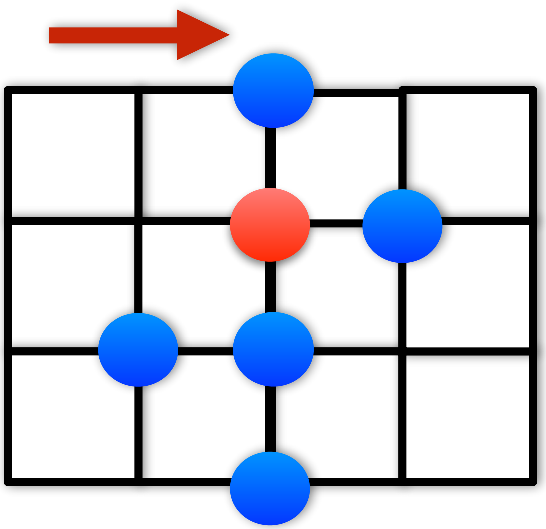
(Leitmann & Franoch, Bénichou et al.)

$$p_\uparrow = p_\downarrow = \frac{1}{4}$$ 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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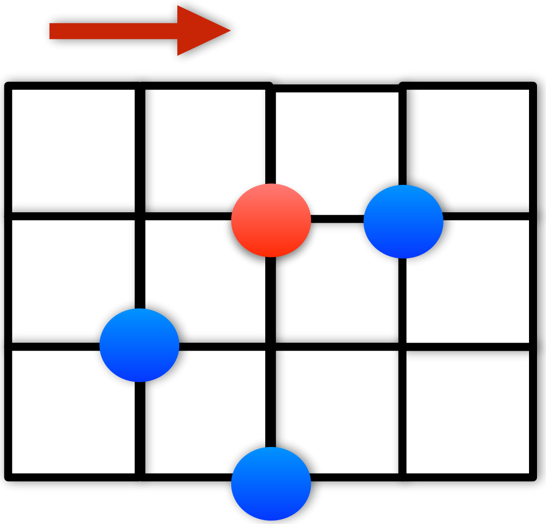

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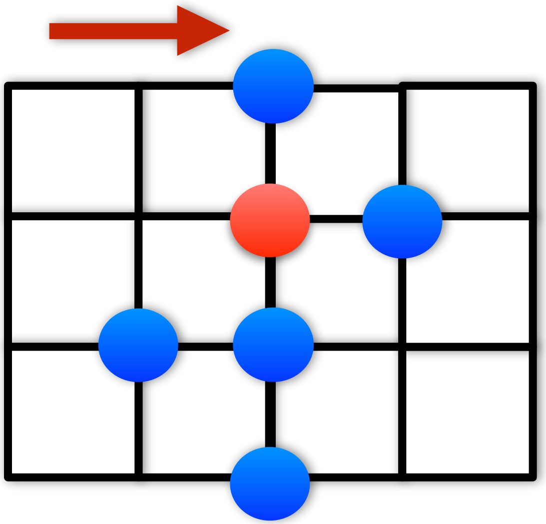


No trapping effect at linear order in the density

Different choices ⟹ significant macroscopic differences

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

(e.g. molecular motors with external load)

Fluctuation-Dissipation Relation

Linear response around nonequilibrium

Trajectory $\omega \equiv \{\boldsymbol{x}_s\}_{s=0}^{s=t}$ characterized by discrete jumps at s_i

and by exponentially distributed waiting times $s_{i+1} - s_i$

Entropy flux $\Sigma(\omega) = \sum_i S(\boldsymbol{x}_{s_i}, \boldsymbol{x}_{s_{i+1}})$

Dynamical activity ("frenesy") $D(\omega) = \int_0^t ds \left(\sum_{\boldsymbol{y}} k(\boldsymbol{x}_s, \boldsymbol{y}) \right) - \sum_i \log \psi(\boldsymbol{x}_{s_i}, \boldsymbol{x}_{s_{i+1}})$

Nonequilibrium FDR $\Rightarrow$ $$\frac{d\langle O \rangle_F}{dF} = \frac{1}{2} \left\langle O \frac{d\Sigma}{dF} \right\rangle_F - \left\langle O \frac{dD}{dF} \right\rangle_F$$

(Baiesi, Maes, Wynants PRL 2009)

Fluctuation-Dissipation Relation

In our case:

jumps on the right

jumps on the left

$$
\begin{aligned}
\Sigma(\omega) &= \beta F(N_{\rightarrow} - N_{\leftarrow}) \\
D(\omega) &= \int_0^t ds \Big\{ p_1[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_1)] + p_{-1}[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_{-1})] \\
&+ p_2[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_2)] + p_{-2}[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_{-2})] \Big\} \\
&- N \log[1/(e^{\beta F/2} + e^{-\beta F/2} + 2)]
\end{aligned}
$$

total number of jumps

Fluctuation-Dissipation Relation

In our case: jumps on the right, jumps on the left

$$\begin{aligned}\Sigma(\omega) &= \beta F(N_{\rightarrow} - N_{\leftarrow}) \\ D(\omega) &= \int_0^t ds \Big\{ p_1[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_1)] + p_{-1}[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_{-1})] \\ &+ p_2[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_2)] + p_{-2}[1-\eta(\boldsymbol{x}_s+\boldsymbol{e}_{-2})] \Big\} \\ &- N \log[1/(e^{\beta F/2} + e^{-\beta F/2} + 2)]\end{aligned}$$

total number of jumps

Consider $O \equiv V$ in $\dfrac{d\langle O\rangle_F}{dF} = \dfrac{1}{2}\left\langle O \dfrac{d\Sigma}{dF}\right\rangle_F - \left\langle O \dfrac{dD}{dF}\right\rangle_F$

Differential mobility, linear response around nonequilibrium

$$\begin{aligned}\frac{d\langle V\rangle_F}{dF} &= \frac{\beta}{2}\langle V^2\rangle_{F,c} - p_1' \langle V\cdot(t-t_{\rightarrow})\rangle_{F,c} - p_{-1}' \langle V\cdot(t-t_{\leftarrow})\rangle_{F,c} \\ &- 2p_2' \langle V\cdot(t-t_{\uparrow})\rangle_{F,c} - h' \langle V\cdot N\rangle_{F,c}\end{aligned}$$

Conclusions

- Microscopic theory for NDM in a driven lattice gas model:
  - ☑ Decoupling approximation
  - ☑ General expression for the force-velocity relation
  - ☑ Exact at low and high density
  - ☑ Unification of recent results

- Criterion for NDM in the parameter space:
  - ☑ Coupling between density and diffusion time scales

- Role of transition rates out of equilibrium
  - ☑ Significant macroscopic effects

Perspectives

- Analytical expression of velocity fluctuations and higher order moments
  - How to infer the applied force from a velocity measurement?
- Nonequilibrium fluctuation-dissipation relations
  - Linear FDR around nonequilibrium
  - Analytical expressions for the terms responsible for NDM

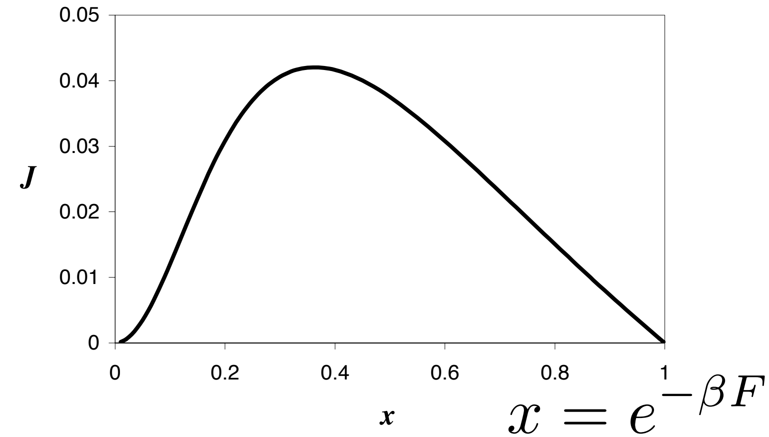
Perspectives

- Analytical expression of velocity fluctuations and higher order moments
  - How to infer the applied force from a velocity measurement?
- Nonequilibrium fluctuation-dissipation relations
  - Linear FDR around nonequilibrium
  - Analytical expressions for the terms responsible for NDM
- Is it possible to observe NDM in off-lattice systems?
  - Recent studies show a monotonic behavior
  - To explore a wider range of parameters (for tracer and obstacles)
- Experiments and simulations in driven granular systems?
- Role of the kinetic part of transition rates out of equilibrium
  - To measure “effective” transition rates from molecular dynamics

Negative differential mobility in different systems

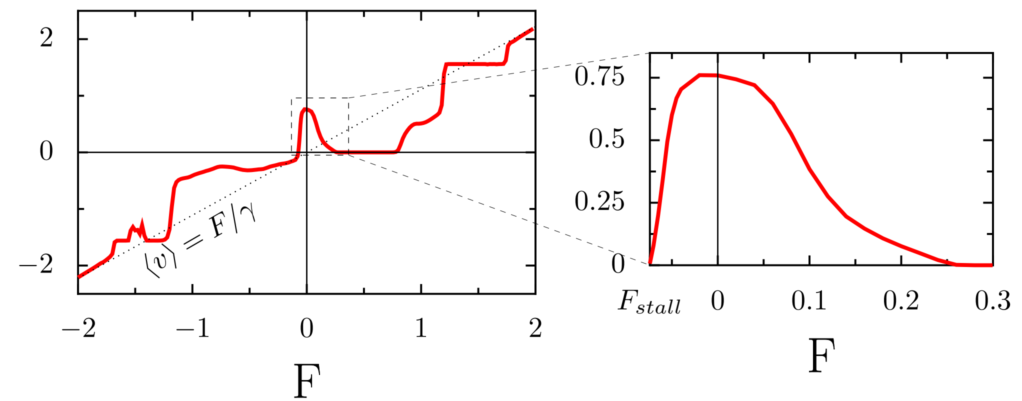
- Nonequilibrium steady states

(Zia et al. Am. J. Phys. 2002)



- Models of Brownian motors

(Cecchi & Magnasco PRL 1996, Kostur et al. Physica A 2006)



- Kinetically constraint models for glassy dynamics

(Jack et al. PRE 2008, Sellitto PRL 2008)