Microscopic Theory for the Diffusion of an Active Particle in a Crowded Environment

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Phys. Rev. Lett. **113**, 268002 (2014)
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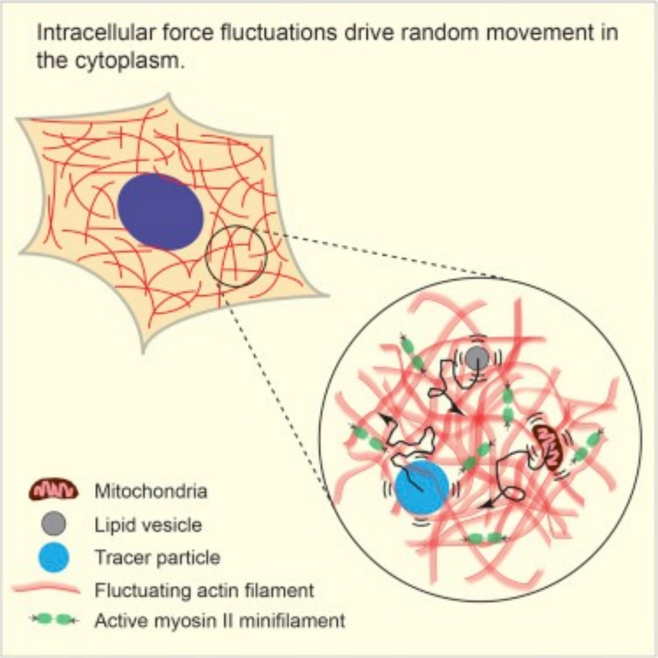
P. Rizkallah , AS, O. Bénichou, P. Illien,
Phys. Rev. Lett. **128**, 038001 (2022)
preprint arXiv: 2212.01216 (2022)

Motivations

To understand the interactions between active particles and complex environments

Transport of biological objects takes place under crowded conditions



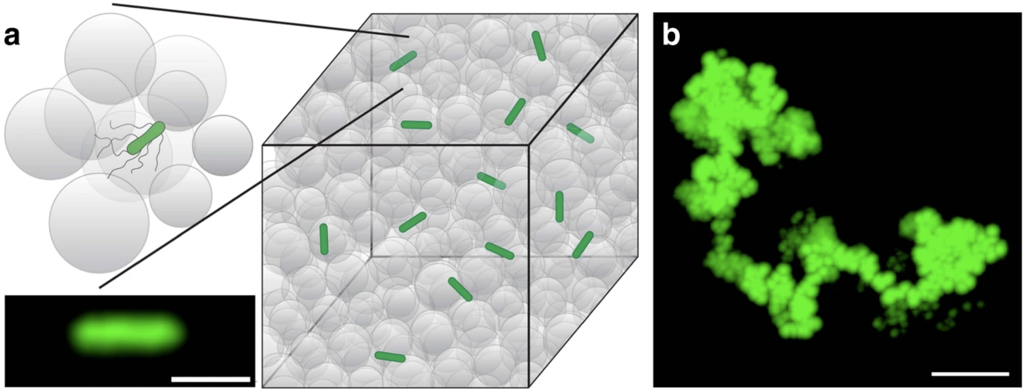
Motor proteins inside a cell

L. Conway, D. Wood, E. Tüzel, and J. L. Ross, Proc. Natl. Acad. Sci. U.S.A. 109, 20814 (2012)

Bacteria in porous materials

N. A. Licata, B. Mohari, C. Fuqua, and S. Setayeshgar, Biophys. J. 110, 247 (2016)

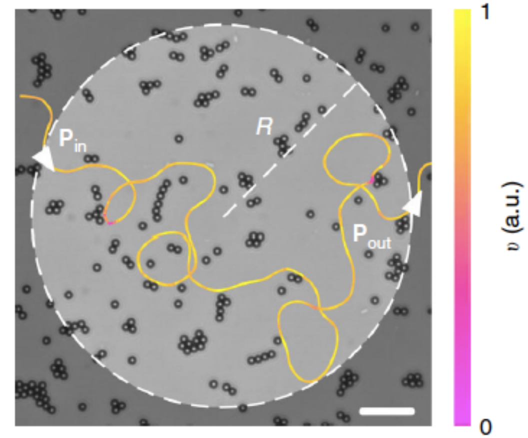
T. Bhattacharjee and S. S. Datta, Nat. Commun. 10, 2075 (2019)



E. coli dispersed in jammed packings of hydrogel particles

Diffusion in crowded environment

Some results in frozen disordered environments



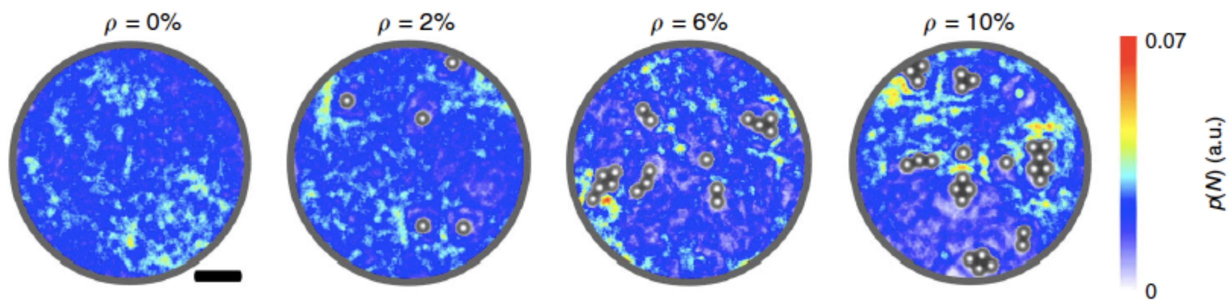
S. Makarchuk, V. C. Braz, N. A. Araújo, L. Ciric, and G. Volpe,
Nat. Commun. 10, 4110 (2019)

O. Sipos, K. Nagy, R. Di Leonardo, and P. Galajda,
Phys. Rev. Lett. 114, 258104 (2015)

J. Tailleur and M. E. Cates,
Europhys. Lett. 86, 60002 (2009)

O. Chepizhko and F. Peruani,
Phys. Rev. Lett. 111, 160604 (2013)

A. Kaiser, H. H. Wensink, and H. Löwen,
Phys. Rev. Lett. 108, 268307 (2012)



Propagation and localisation of E. coli cells near surfaces with micro-obstacles

Few (numerical) results in environments of mobile obstacles

M. J. Saxton, Biophys. J. 52, 989 (1987)

N. Dorsaz, et al. Phys. Rev. Lett. 105, 120601 (2010)

J. D. Schmit, E. Kamber, and J. Kondev,
Phys. Rev. Lett. 102, 218302 (2009)

Theory by Nakazato and Kitahara

Case of a passive tracer: theory by Nakazato and Kitahara for a lattice gas

Diffusion coefficient as a function of the density of crowders

$$D = \frac{1}{2d\tau}(1-\rho)\left[1 - \frac{2\rho\frac{\tau^*}{\tau}\gamma}{2d\left[1+\frac{\tau^*}{\tau}(1-\rho)\right] - \left[1+\frac{\tau^*}{\tau}(1-3\rho)\gamma\right]}\right]$$

ρ particle density

Many-body nature of the problem

Approximate expression, exact in the low and high density regimes

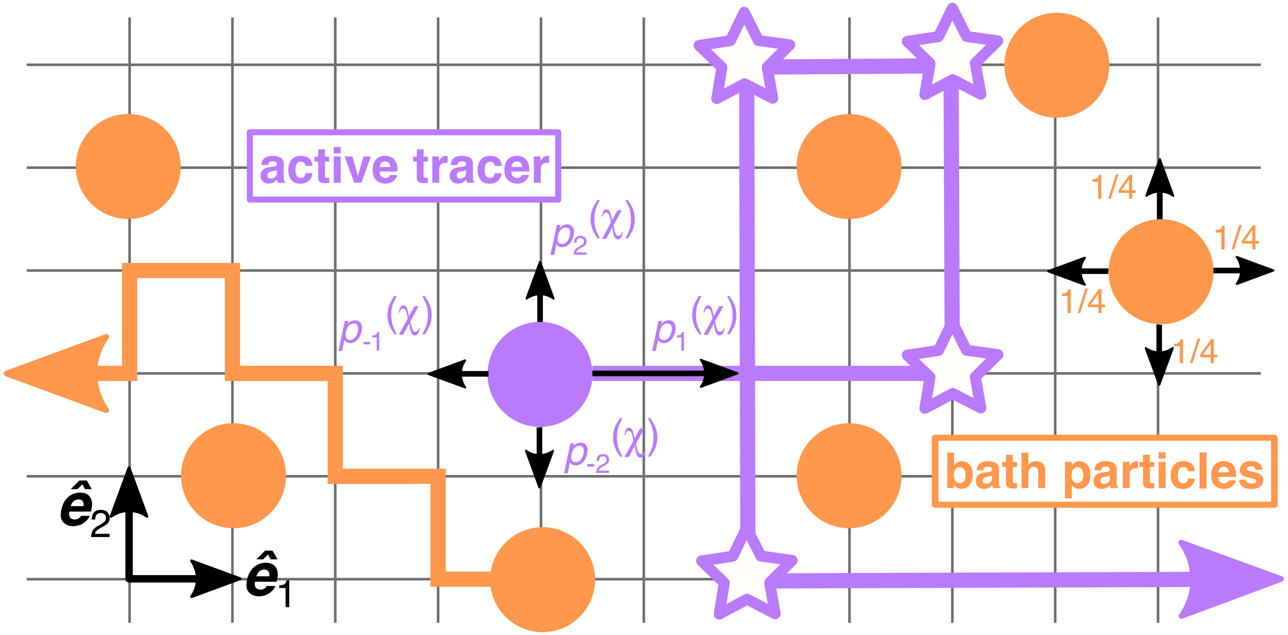
Good quantitative estimates for arbitrary density,
if the environment is mobile enough

K. Nakazato and K. Kitahara,
Prog. Theor. Phys. 64, 2261 (1980)

R. A. Tahir-Kheli and R. J. Elliott,
Phys. Rev. B 27, 844 (1983)

H. van Beijeren and R. Kutner,
Phys. Rev. Lett. 55, 238 (1985)

The model: active particle on a lattice gas



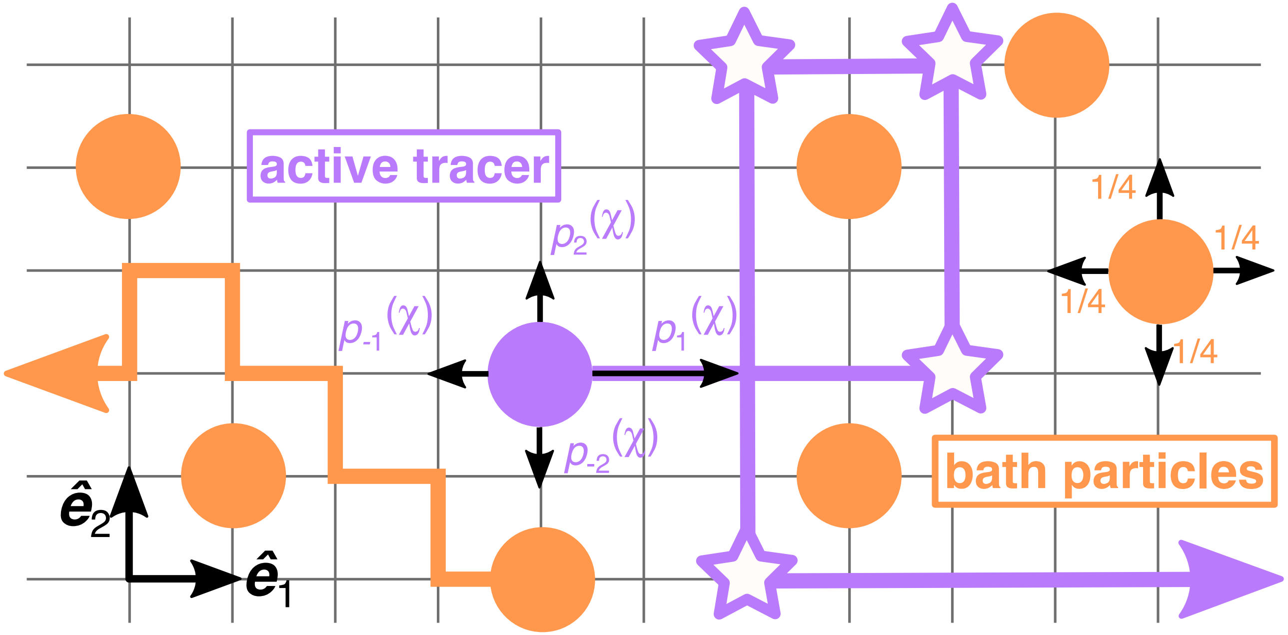
Jump probability

$$p_\mu^{(\chi)} \propto e^{\frac{F_A \boldsymbol{e}_\chi \cdot \boldsymbol{e}_\mu}{2}}$$

Active particle driven by a force F_A, asymmetric exclusion process, average waiting time τ

Persistence time $\tau_\alpha = 2d\tau^*/\alpha$ in the state χ

The model: active particle on a lattice gas



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N hard-core particles in d dimensions, symmetric exclusion process, average waiting time τ^*

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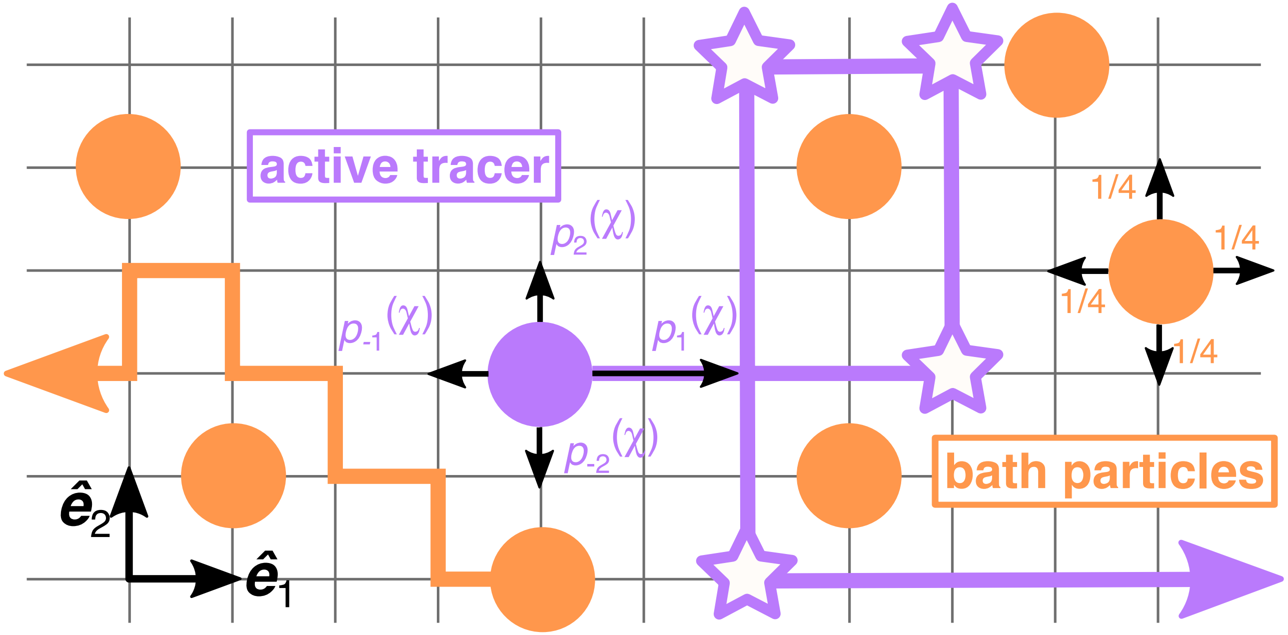

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Active particle driven by a force F_A, asymmetric exclusion process, average waiting time τ

Persistence time $\tau_\alpha = 2d\tau^*/\alpha$ in the state χ

N hard-core particles in d dimensions, symmetric exclusion process, average waiting time τ^*

The dynamics of the tracer is a lattice representation of a run-and-tumble dynamics

Master Equation

The dynamics of the model is described by a Master Equation

$$2d\tau^*\partial_t P_\chi(\mathbf{R},\eta;t) = \mathcal{L}_\chi P_\chi - \alpha P_\chi + \frac{\alpha}{2d-1}\sum_{\chi'\neq\chi} P_{\chi'}$$

$P_\chi(\mathbf{R},\eta;t)$ joint probability to find the tracer in state χ, at site $\mathbf{R}$, with the lattice in configuration $\eta = \{\eta_\mathbf{r}\}$ the system at time t

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$\mathcal{L}_\chi$ evolution operator in state χ

$$\mathcal{L}_\chi P_\chi = \sum_{\nu=1}^{d}\sum_{\boldsymbol{r}\neq\boldsymbol{R}-\boldsymbol{e}_\nu,\boldsymbol{R}} \left[P_\chi(\boldsymbol{R},\eta^{\boldsymbol{r},\nu};t) - P_\chi(\boldsymbol{R},\eta;t)\right]$$ evolution of bath particles

$$+\frac{2d\tau^*}{\tau}\sum_\mu p_\mu^{(\chi)}\left[(1-\eta_{\boldsymbol{R}})\,P_\chi(\boldsymbol{R}-\boldsymbol{e}_\mu,\eta;t) - \left(1-\eta_{\boldsymbol{R}+\boldsymbol{e}_\mu}\right)P_\chi(\boldsymbol{R},\eta;t)\right]$$

evolution of the tracer

Diffusion coefficient

Expression for the diffusion coefficient $D \equiv \lim_{t\to\infty} \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle X_t^2 \rangle$

$$D = \frac{1}{4d\tau}\sum_{\chi}\sum_{\epsilon=\pm 1}\left\{p_\epsilon^{(\chi)}\left[1-k_\epsilon^{(\chi)}\right] - 2\epsilon p_\epsilon^{(\chi)}\widetilde{g}_\epsilon^{(\chi)}\right\}$$

$$+\frac{2d-1}{2d}\frac{\tau^*}{\tau^2\alpha}\sum_{\chi}\left\{\sum_{\epsilon=\pm 1}\epsilon p_\epsilon^{(\chi)}\left[1-k_\epsilon^{(\chi)}\right]\right\}^2$$

$k_{\boldsymbol{r}}^{(\chi)} = \langle \eta_{\boldsymbol{X}_t+\boldsymbol{r}} \rangle_\chi$ density profiles in the frame of reference of the tracer

$\widetilde{g}_{\boldsymbol{r}}^{(\chi)} = \langle \eta_{\boldsymbol{X}_t+\boldsymbol{r}}(X_t - \langle X_t \rangle_\chi) \rangle_\chi$ tracer-bath cross-correlations functions

$\langle\cdot\rangle_\chi = 2d\sum_{\boldsymbol{R},\eta}\cdot P_\chi(\boldsymbol{R},\eta;t)$ average conditioned on state χ

Decoupling approximation

Equations for the density profile $k_{\mathbf{r}}^{(\chi)}$ and for the tracer-bath cross-correlation $\tilde{g}_{\mathbf{r}}^{(\chi)}$ are not closed and involve higher-order correlation functions

Closure scheme, mean-field-like approximation

$$\langle \eta_{\mathbf{r}} \eta_{\mathbf{r}'} \rangle_{\chi} \simeq k_{\mathbf{r}}^{(\chi)} k_{\mathbf{r}'}^{(\chi)}$$

$$\langle \delta X_t \eta_{\mathbf{r}} \eta_{\mathbf{r}'} \rangle_{\chi} \simeq k_{\mathbf{r}}^{(\chi)} \tilde{g}_{\mathbf{r}'}^{(\chi)}$$

Coupled dynamical equations

We obtain the following equations for $h_{\boldsymbol{r}}^{(\chi)} \equiv k_{\boldsymbol{r}}^{(\chi)} - \rho$ (defined in such a way that $\lim_{|\boldsymbol{r}|\to\infty} h_{\boldsymbol{r}} = 0$) and $\tilde{g}_{\boldsymbol{r}}^{(\chi)}$ (we adopt the convention $h_{\boldsymbol{0}}^{(\chi)} = \tilde{g}_{\boldsymbol{0}}^{(\chi)} = 0$)

Density profile evolution equation

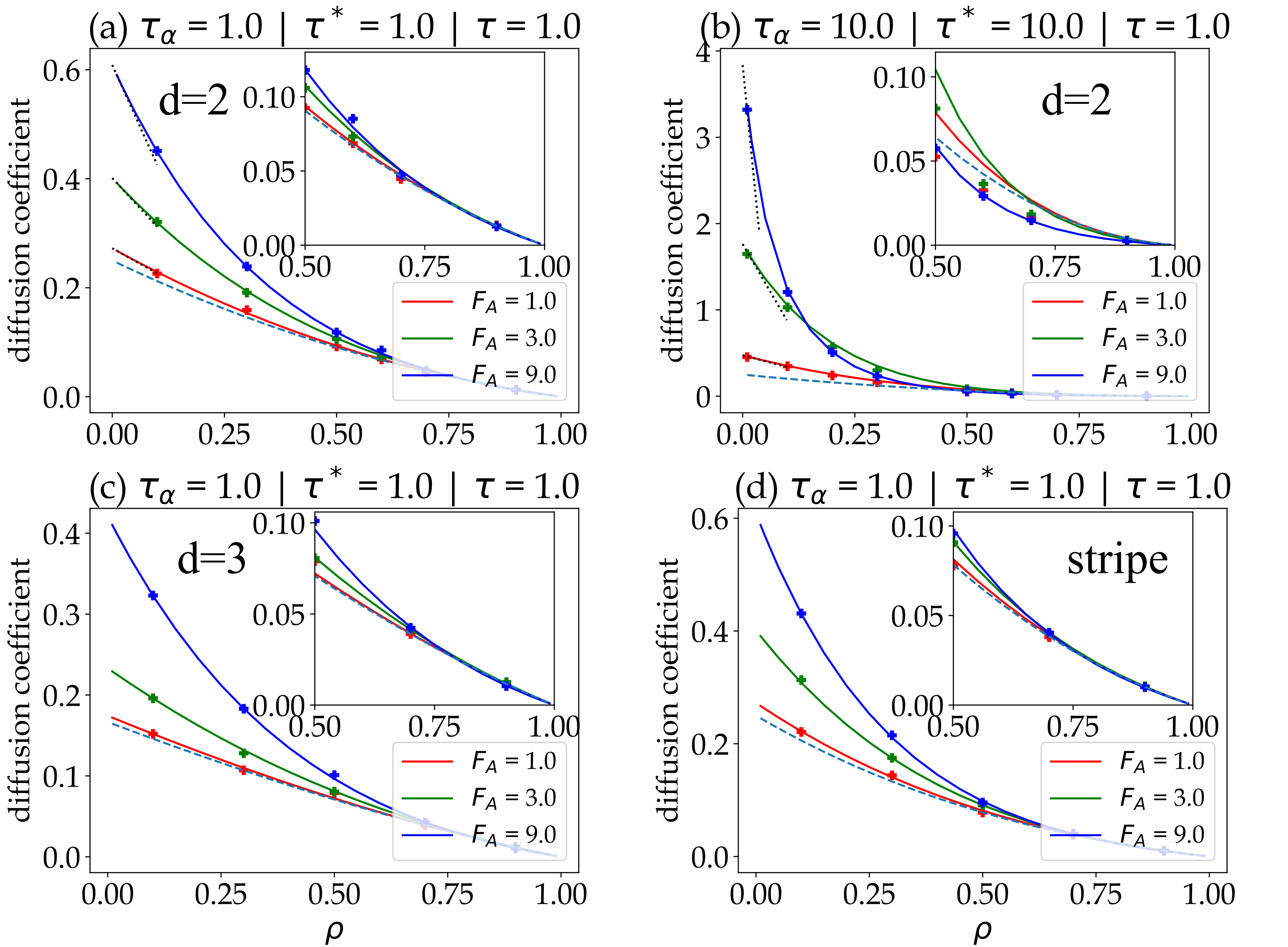
$$2d\tau^*\partial_t h_{\boldsymbol{r}}^{(\chi)} = (\tilde{L}^{(\chi)} + \sum_\nu A_\nu^{(\chi)} \delta_{\boldsymbol{r},\boldsymbol{e}_\nu}) h_{\boldsymbol{r}}^{(\chi)} + \sum_\nu \delta_{\boldsymbol{r},\boldsymbol{e}_\nu} \rho (A_\nu - A_{-\nu}) - \alpha h_{\boldsymbol{r}}^{(\chi)} + \frac{\alpha}{2d-1} \sum_{\chi' \neq \chi} h_{\boldsymbol{r}}^{(\chi')}, \quad (3)$$

Tracer-bath cross correlation function

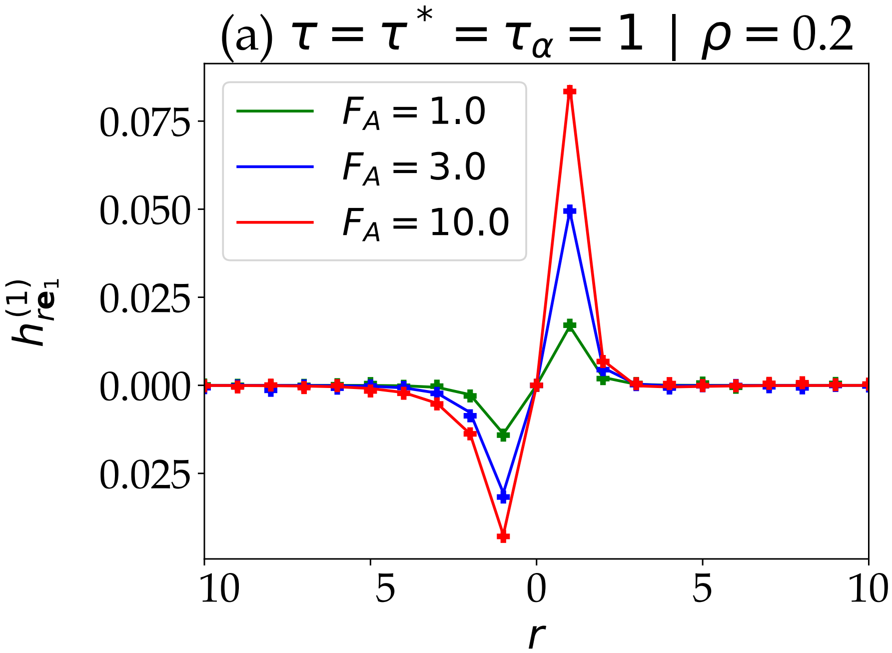
$$2d\tau^*\partial_t \tilde{g}_{\boldsymbol{r}}^{(\chi)} = \left(\tilde{L}^{(\chi)} + \sum_\nu A_\nu^{(\chi)} \delta_{\boldsymbol{r},\boldsymbol{e}_\nu}\right) \tilde{g}_{\boldsymbol{r}}^{(\chi)} + \mathcal{G}^{(\chi)} h_{\boldsymbol{r}}^{(\chi)} - \alpha \tilde{g}_{\boldsymbol{r}}^{(\chi)} + \frac{\alpha}{2d-1} \sum_{\chi' \neq \chi} \tilde{g}_{\boldsymbol{r}}^{(\chi')} + \sum_\nu \delta_{\boldsymbol{r},\boldsymbol{e}_\nu} [(A_{-\nu}^{(\chi)} - 1)\rho(\boldsymbol{e}_\nu \cdot \boldsymbol{e}_1) - \frac{2d\tau^*}{\tau}(p_\nu^{(\chi)} \tilde{g}_{\boldsymbol{e}_\nu}^{(\chi)} (h_{\boldsymbol{e}_\nu}^{(\chi)} + \rho) - \rho p_{-\nu}^{(\chi)} \tilde{g}_{\boldsymbol{e}_{-\nu}}^{(\chi)})], \quad (4)$$

where we define $A_\mu^{(\chi)} \equiv 1 + (2d\tau^*/\tau) p_\mu^{(\chi)} [1 - k_{\boldsymbol{e}_\mu}^{(\chi)}]$, the operator $\tilde{L}^{(\chi)}$ acting on a test function $f_{\boldsymbol{r}}$ as $\tilde{L}^{(\chi)} f_{\boldsymbol{r}} \equiv \sum_\mu A_\mu^{(\chi)} (f_{\boldsymbol{r}+\boldsymbol{e}_\mu} - f_{\boldsymbol{r}})$.

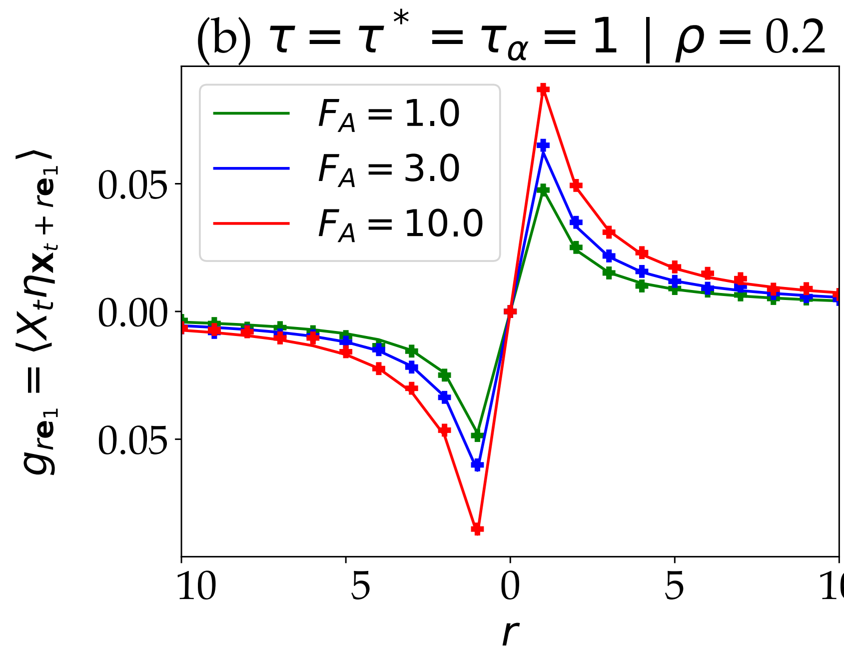
Diffusion coefficient: comparison with MC simulations



Density profiles



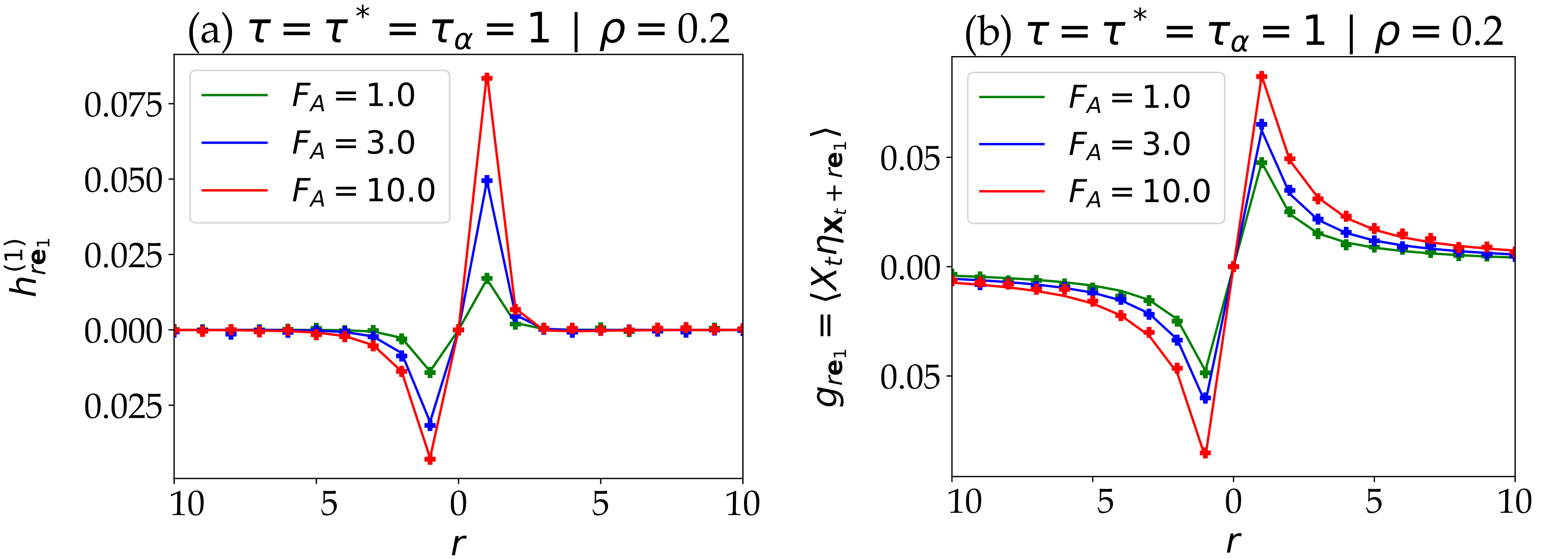
density profile



tracer-bath correlation function

→ Interplay between the displacement of the active particle and the response of the environment

Density profiles

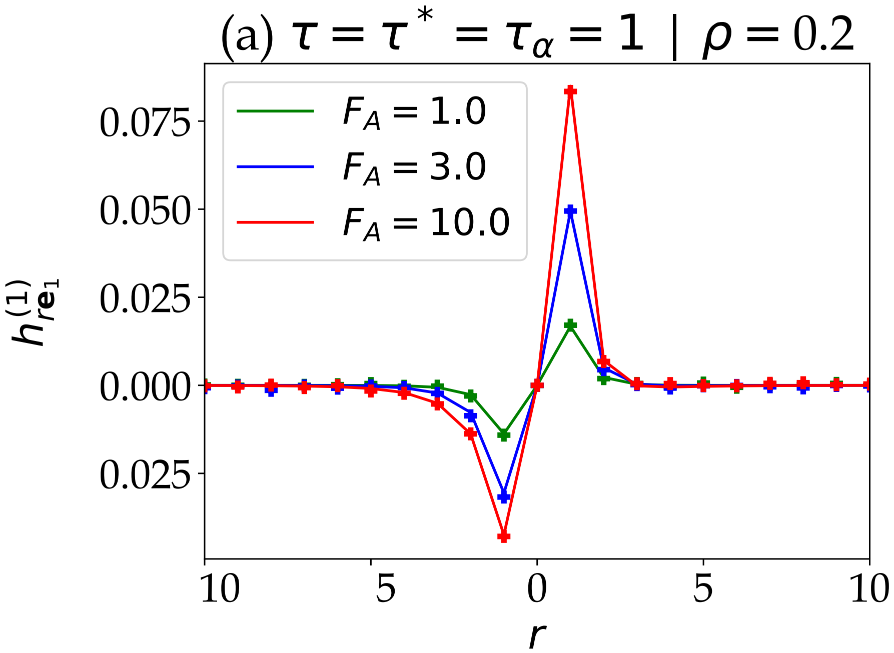


density profile

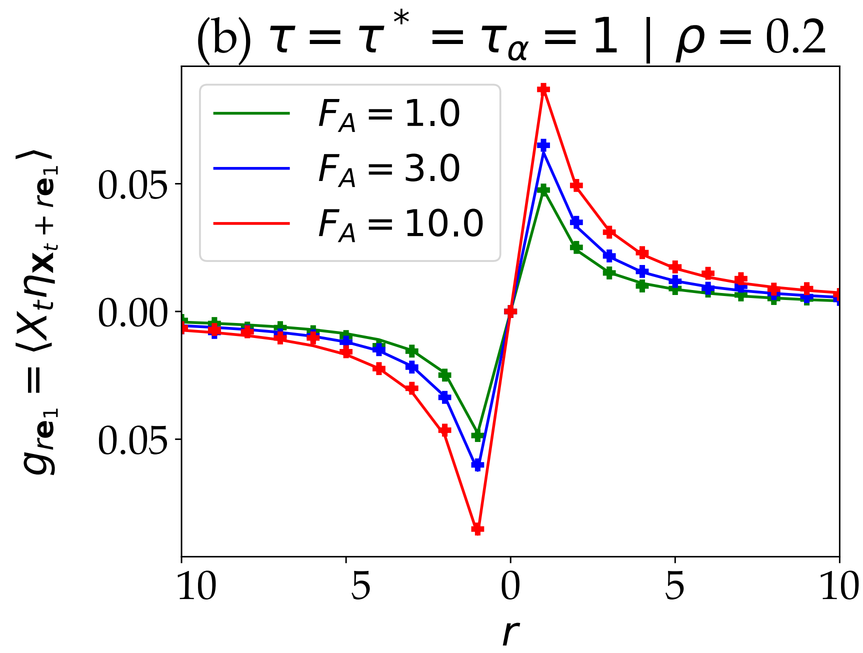
tracer-bath correlation function

- Interplay between the displacement of the active particle and the response of the environment
- Accumulation of bath particles in front of the tracer and depletion behind it

Density profiles



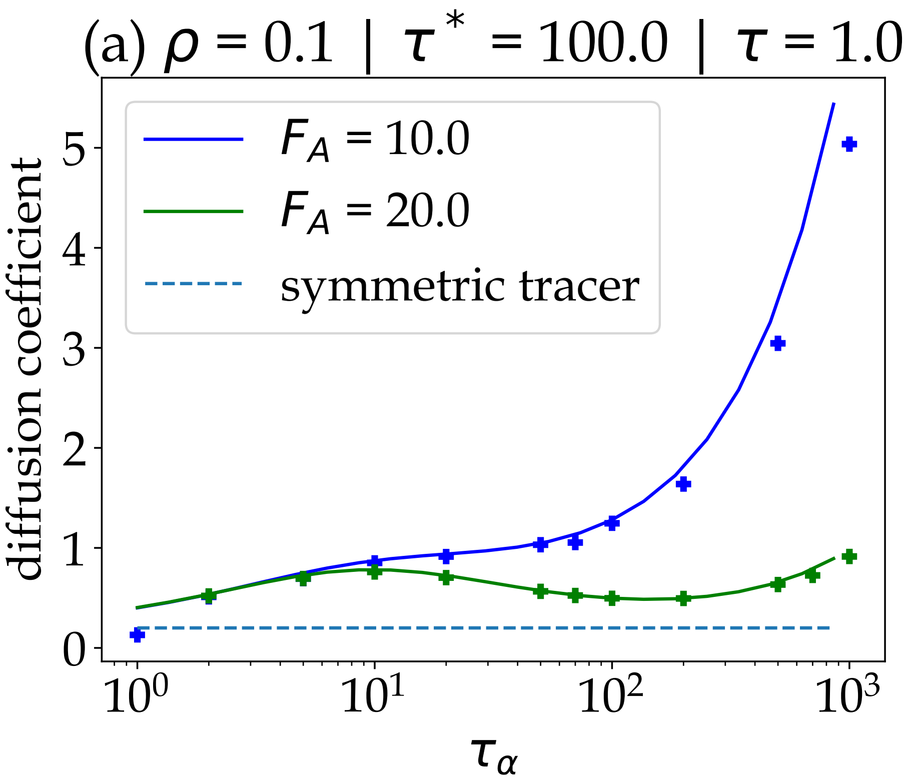
density profile

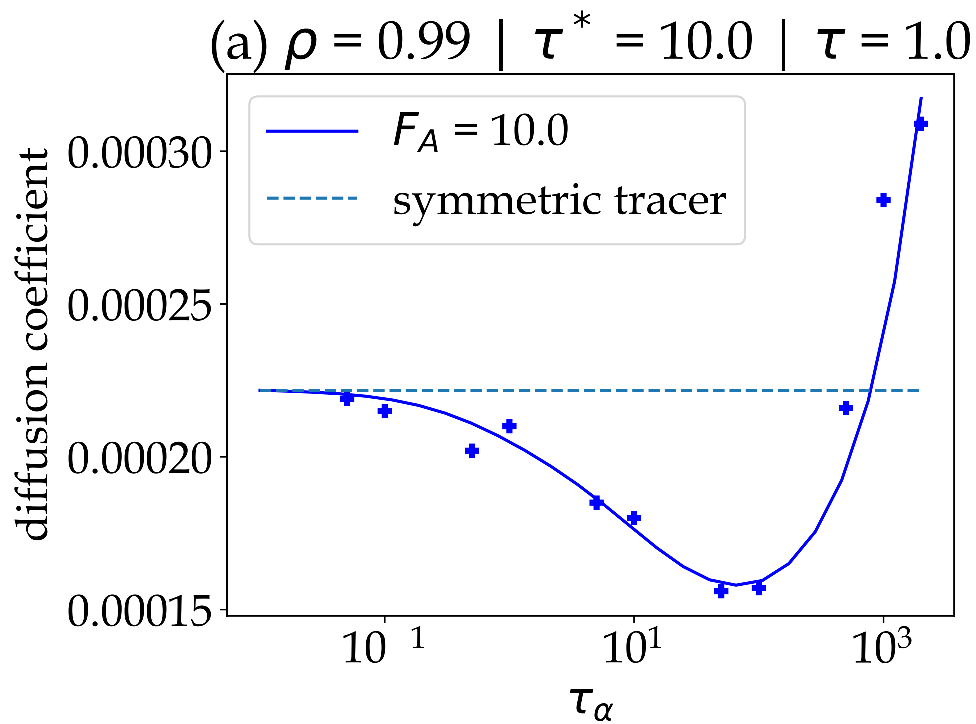


tracer-bath correlation function

- Interplay between the displacement of the active particle and the response of the environment
- Accumulation of bath particles in front of the tracer and depletion behind it
- Local anisotropy of the environment induced by the active particle

Non-monotonic behaviour of the diffusion coefficient





Asymptotic limits:

$\tau_\alpha \to 0$ passive (symmetric) tracer (NK theory)

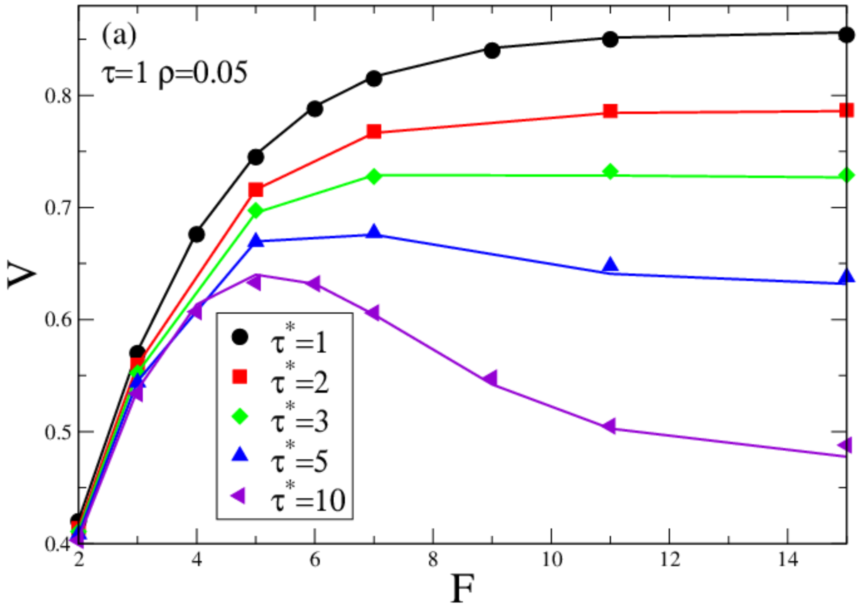
$\tau_\alpha \to \infty$ diffusion coefficient diverges (except in the specific limit of fixed obstacles)

Non-monotonic behaviour between these two limits

Driven passive particle

Apply an external force on the passive tracer

Negative differential mobility can be observed



Bénichou, AS, et al. Phys. Rev. Lett. (2014)
Phys. Rev. E (2016)

Baiesi et al. Phys. Rev. E 92, 042121 (2015)

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

"Getting more from pushing less" Zia et al. Am. J. Phys. (2002)

Driven active particle

Apply an external force on the active particle

$$p_\mu^{(\chi)} = \frac{\exp\left[(F_A\mathbf{e}_\chi + F_E\mathbf{e}_1)\cdot\mathbf{e}_\mu/2\right]}{Z}$$

Tracer velocity

$$\frac{\mathrm{d}\langle X_t\rangle}{\mathrm{d}t} = \frac{1}{2d\tau}\sum_\chi \left\{p_1^{(\chi)}\left[1-k_{\boldsymbol{e}_1}^{(\chi)}\right] - p_{-1}^{(\chi)}\left[1-k_{\boldsymbol{e}_{-1}}^{(\chi)}\right]\right\}$$

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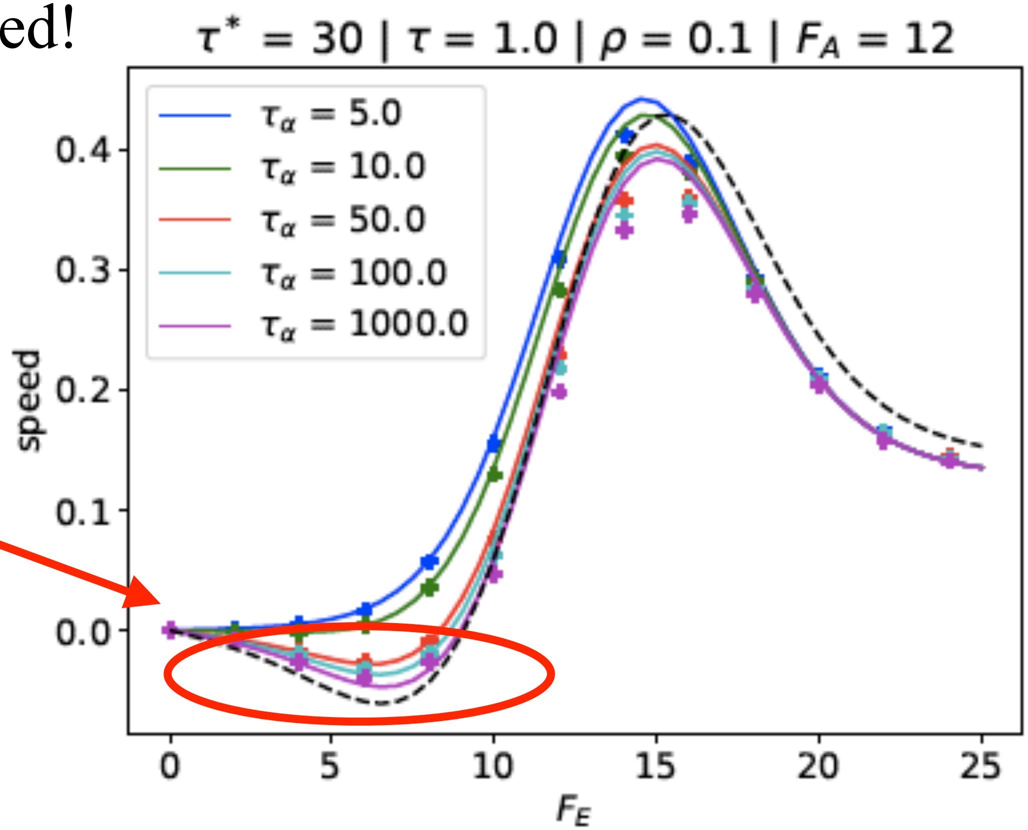
Negative mobility can be observed!

Absolute negative mobility!



Conclusions

Interest in lattice gas models for active particles

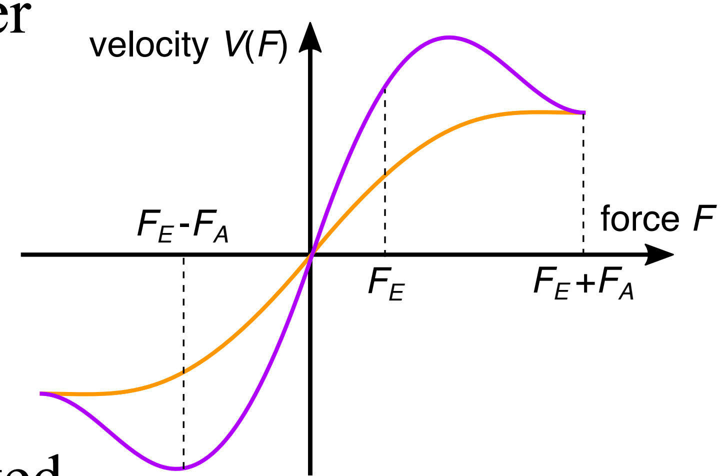
Analytical treatment in the interacting case is possible (with some approximations)

Coupling between active tracer and environment, response of the medium

Nonlinear striking effects are observed: non-monotonic behaviours, optimal parameters to maximise/minimise diffusion (or mobility), absolute negative mobility

Simple argument for ANM

Consider the simple situation where the tracer is submitted to an active force F_A that may only point in directions ± 1



In the limit where the persistence time is greater than other timescales, the average velocity of the tracer can therefore be estimated as the average of the velocities conditioned on these two states $V \simeq \dfrac{1}{2}[V_0(F_E + F_A) + V_0(F_E - F_A)]$,

where $V_0(F)$ is the stationary velocity of a passive particle submitted to an external force F

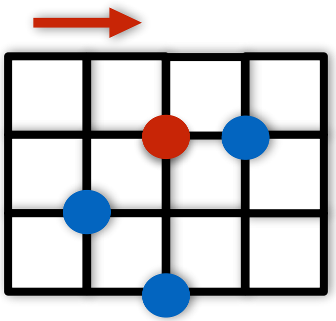
When the tracer displays negative differential mobility, one may observe the situation where $|V_0(F_E - F_A)| > |V_0(F_E + F_A)|$, therefore resulting in a situation where average velocity V is negative although $F_E > 0$.

Simple arguments for the non-monotony of D

Assume low density and large active force

The obstacles are independent and the probability for the tracer to find an obstacle at a given site is ρ

For a large force $F \to \infty$, neglect the probability that the tracer moves in the direction opposite to the force



Approximate the characteristic time between two jumps as:
internal jump time τ + the mean trapping time;
the escape from a trap is caused by three independent events:
— the obstacle moves in a transverse direction with characteristic time τ*;
— the active force changes direction with characteristic time τα;
— the tracer moves in a direction transverse to the active force with characteristic time $\tau/(1-p_{\chi}^{(x)}-p_{-\chi}^{(x)})$.

Mean trapping time $$\frac{1}{\tau_p} = \frac{(2d-2)}{2d\tau^*} + \frac{1}{\tau_\alpha} + \frac{(1-p_1^{(1)}-p_{-1}^{(1)})}{\tau}$$

Diffusion coefficient $$D = \frac{1}{2d(\tau+\rho\tau_p)}\left[1 + \frac{(2d-1)\tau_\alpha}{d(\tau+\rho\tau_p)}\left(p_1^{(1)}-p_{-1}^{(1)}\right)^2\right]$$