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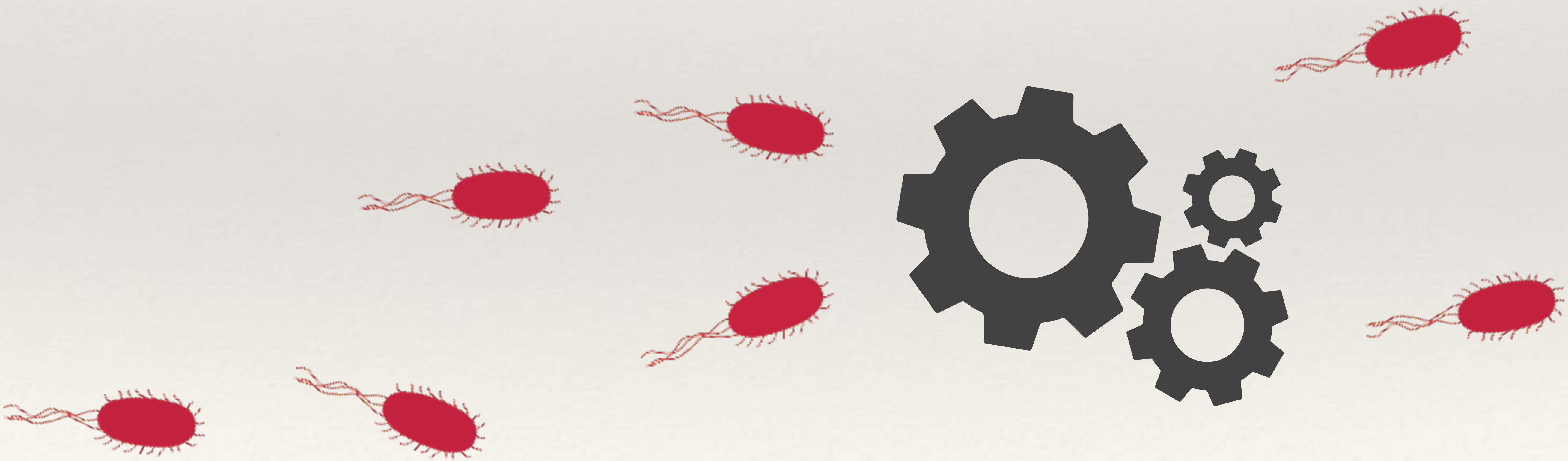
A systematic Markovian approximation method for weakly active particles

Yongjoo Baek
Seoul National University

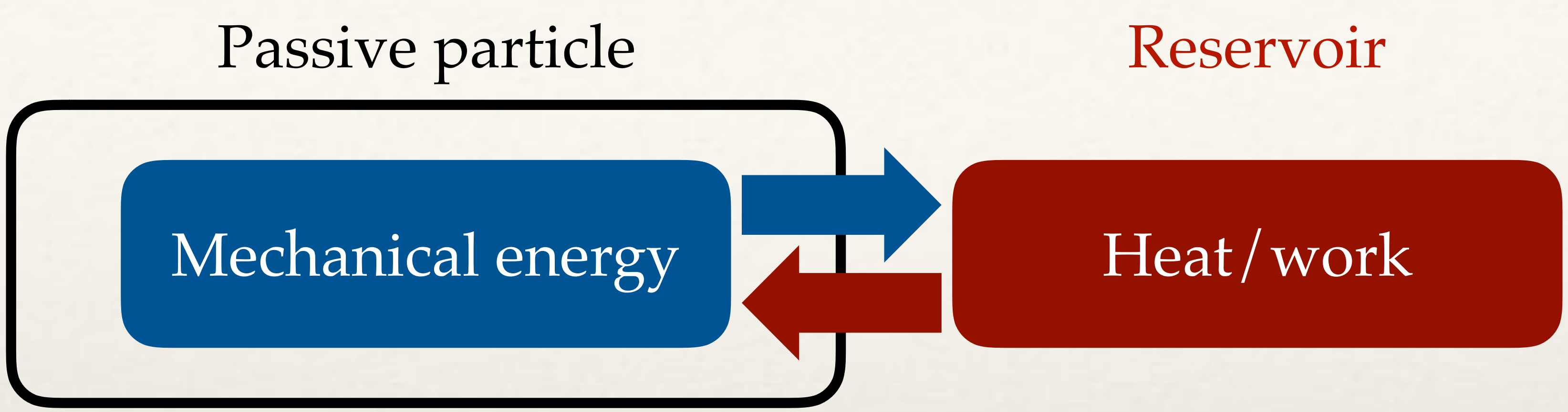
Zigan Zhen, Michael E. Cates
University of Cambridge



Outline

- An active particle as a Brownian particle driven by Gaussian colored noise
- Simple Markovian approximation: “UCNA”
  - Application to motility-induced phase separation
- Systematic Markovian approximation
  - Application to non-equilibrium currents and long-range effects
- Implications

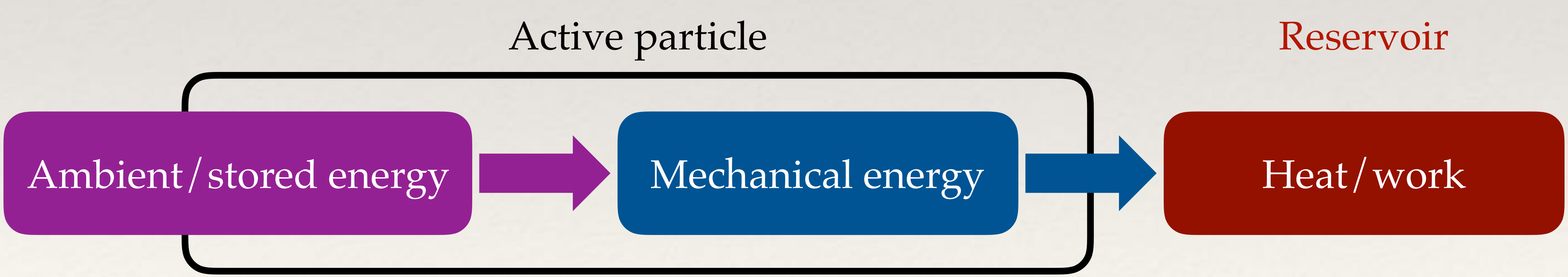
Passive vs. Active



$$K * \dot{\hat{x}} = -V'(\hat{x}) + \hat{\eta}$$

Fluctuation-Dissipation Theorem (FDT)

$$\langle \hat{\eta}(t)\hat{\eta}(s)\rangle = TK(|t-s|)$$



$$K * \dot{\hat{x}} = -V'(\hat{x}) + \hat{v}$$

No FDT $\langle \hat{v}(t)\hat{v}(s)\rangle \neq TK(|t-s|)$

A simple model of active particles

$$\langle \hat{v}(t)\hat{v}(s)\rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t-s|/\tau}$$

(Self-propulsion as Gaussian colored noise)

$$K * \dot{\hat{x}} = -V'(\hat{x}) + \hat{v}$$

$$K(|t-s|) = 2\delta(t-s)$$

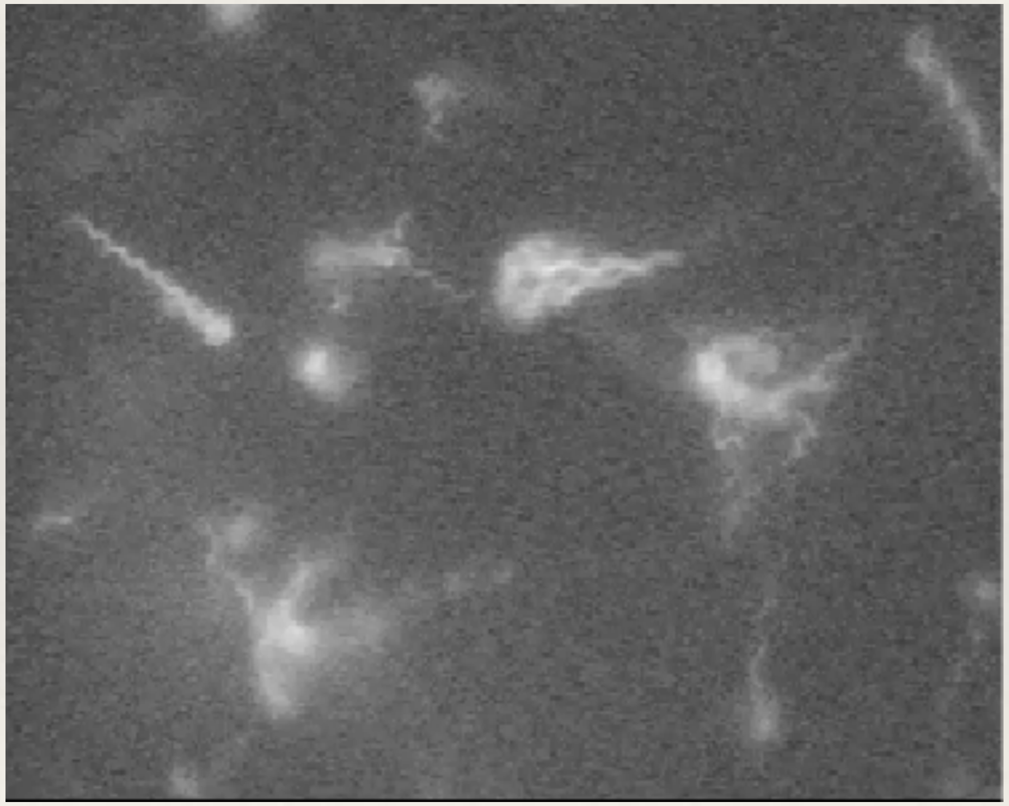
(Fast reservoir at low temperature)

A simple model of active particles

$$\dot{\hat{x}} = -\,V'(\hat{x}) + \hat{v} \qquad \langle \hat{v}(t)\hat{v}(s)\rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t-s|/\tau}$$

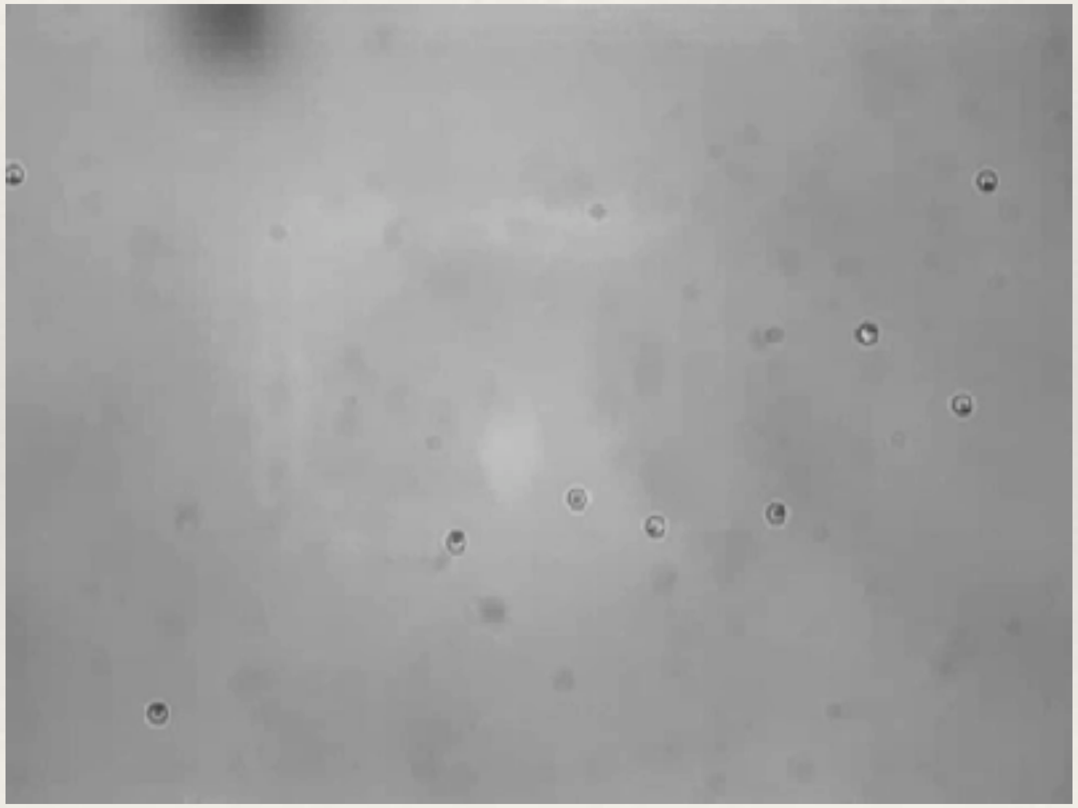
(Self-propulsion as Gaussian colored noise)

Escherichia coli



[from Howard Berg's lab webpage]

Light-activated colloidal surfers



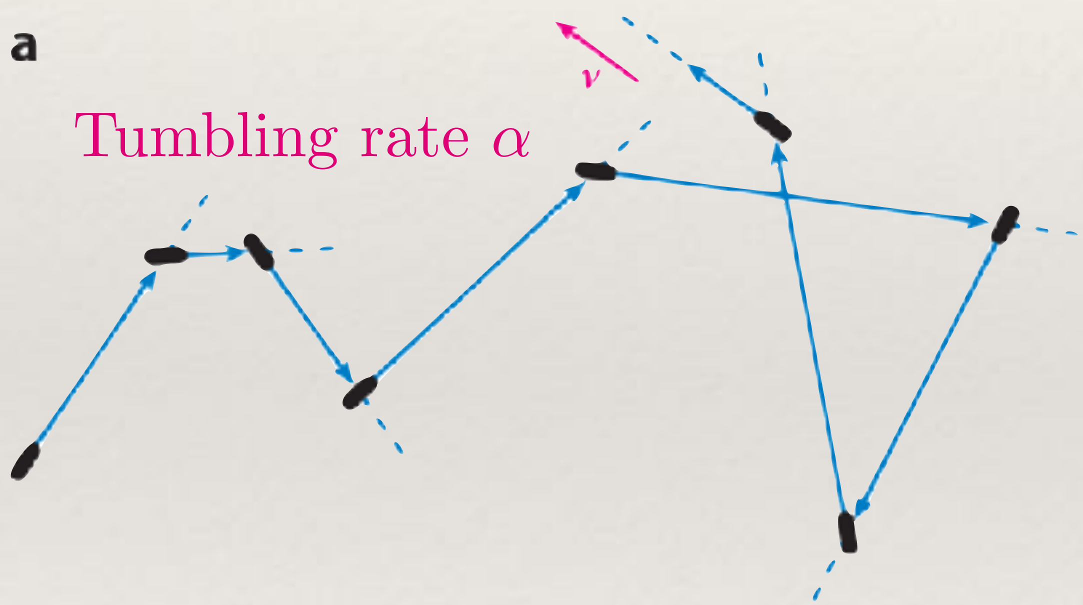
[Palacci *et. al.*, Science **339**, 936 (2013)]

A simple model of active particles

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \qquad \langle \hat{v}(t)\hat{v}(s)\rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t-s|/\tau}$$

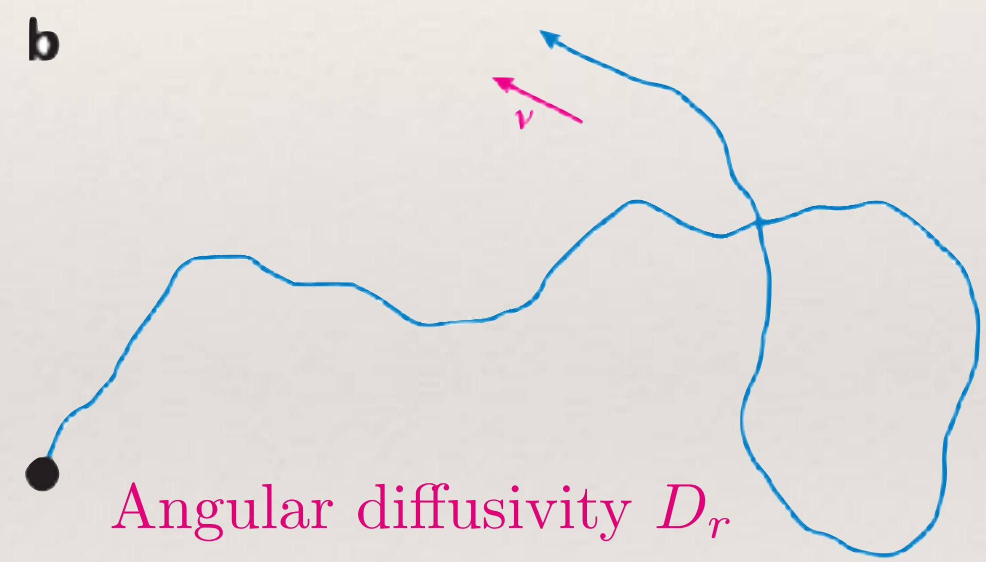
(Self-propulsion as Gaussian colored noise)

Run-and-tumble particles



$$D = \frac{v^2}{2\alpha}, \quad \tau = \frac{1}{\alpha}$$

Active Brownian particles



$$D = \frac{v^2}{2D_r}, \quad \tau = \frac{1}{D_r}$$

A simple model of active particles

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \qquad \langle \hat{v}(t)\hat{v}(s)\rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t-s|/\tau} \xrightarrow[\tau\to 0]{} 2D\delta(t-s)$$

(reduces to EQ dynamics)

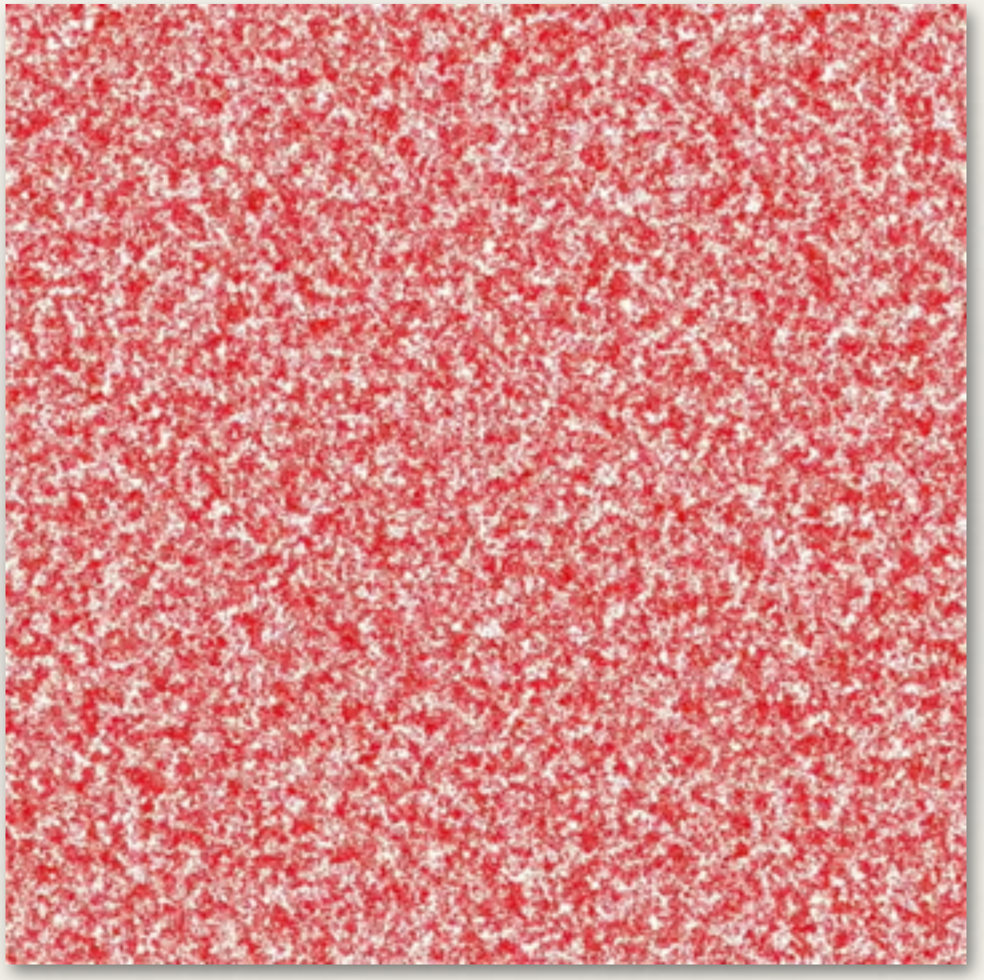
NEQ driving at the level of each particle for nonzero τ.

- **Objective:** identify the NEQ features of active particles by studying the effects of small but nonzero τ through a Markovian approximation.

Phase separation

- Phase separation at EQ requires attractions.
- Short-range repulsion + Self-propelled particles $\Longrightarrow$ Phase separation (No attraction needed!)
- **Motility-Induced Phase Separation (MIPS)**: phase separation due to reduced motility in high-density regions

2D lattice model of bacteria



[Redner, Hagan, & Baskaran, PRL (2013)]

Unified Colored-Noise Approximation (UCNA)

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \qquad \langle \hat{v} \rangle = 0 \qquad \langle \hat{v}(t)\,\hat{v}(s) \rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t-s|/\tau}$$

Colored noise = Ornstein–Uhlenbeck process

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \qquad \dot{\hat{v}} = -\frac{1}{\tau}\hat{v} + \hat{\xi} \qquad \left\langle \hat{\xi} \right\rangle = 0 \qquad \left\langle \hat{\xi}(t)\hat{\xi}(s) \right\rangle = \frac{2D}{\tau^2}\delta(t-s)$$

Elimination of $\hat{v}$

$$\ddot{\hat{x}} = -\frac{1}{\tau}\left[1 + \tau V''(\hat{x})\right] \circ \dot{\hat{x}} - \frac{1}{\tau} V'(\hat{x}) + \hat{\xi}$$

$\ddot{\hat{x}} = 0$

$$\dot{\hat{x}} = -\frac{V'(\hat{x})}{1 + \tau V''(\hat{x})} + \frac{\tau}{1 + \tau V''(\hat{x})} \circ \hat{\xi}$$

Stratonovich product

[Jung & Hänggi, PRA **35**, 44464 (1987)], [Hänggi & Jung, Adv. Chem. Phys. (1994)]

Unified Colored-Noise Approximation (UCNA)

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \qquad \langle \hat{v} \rangle = 0 \qquad \langle \hat{v}(t)\,\hat{v}(s) \rangle = \frac{D}{\tau}\,\mathrm{e}^{-|t-s|/\tau}$$

Colored noise = Ornstein–Uhlenbeck process

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \qquad \dot{\hat{v}} = -\frac{1}{\tau}\hat{v} + \hat{\xi} \qquad \left\langle \hat{\xi} \right\rangle = 0 \qquad \left\langle \hat{\xi}(t)\hat{\xi}(s) \right\rangle = \frac{2D}{\tau^2}\delta(t-s)$$

Elimination of $\hat{v}$

$$\ddot{\hat{x}} = -\frac{1}{\tau}\left[1 + \tau V''(\hat{x})\right] \circ \dot{\hat{x}} - \frac{1}{\tau}V'(\hat{x}) + \hat{\xi}$$

$\ddot{\hat{x}} = 0$

$$\partial_t P = \partial_x \left(\frac{V'P}{1+\tau V''} \right) + D \left(\partial_x \frac{1}{1+\tau V''} \right)^2 P$$

[Jung & Hänggi, PRA **35**, 44464 (1987)], [Hänggi & Jung, Adv. Chem. Phys. (1994)]

Equilibrium-like solutions

$$\partial_t P = \partial_x \left(\frac{V'P}{1+\tau V''} \right) + D \left(\partial_x \frac{1}{1+\tau V''} \right)^2 P$$

has a zero-current steady-state solution

$$P^{\mathrm{s}} \sim \exp\left[-\frac{V}{D} - \tau \left(\frac{V'^2}{2D} - V'' \right) \right]$$

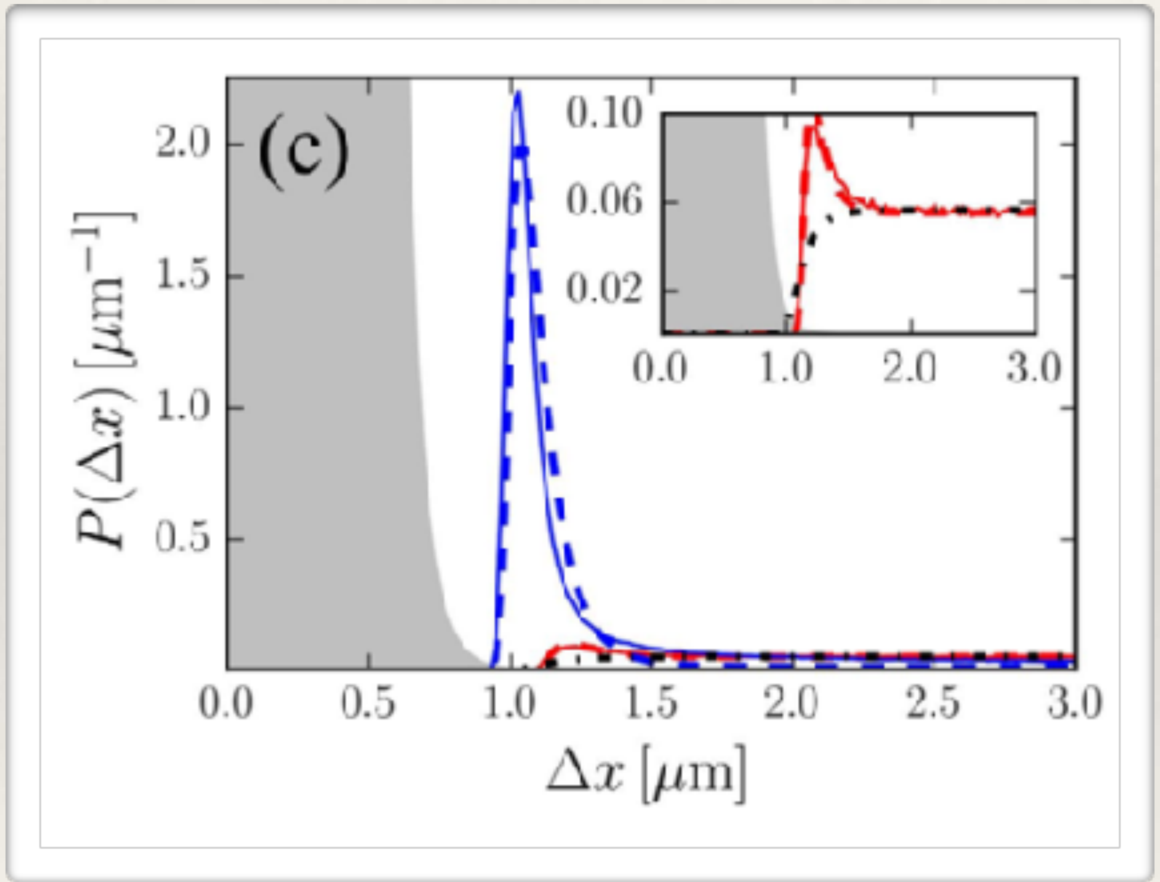
Effective attraction if $V'' > 0$

- Detailed balance holds in the steady state.
- Even repulsive walls can be effectively attractive, allowing high-density clusters to form.
  $\Longrightarrow$ Equilibrium-like mechanism of MIPS

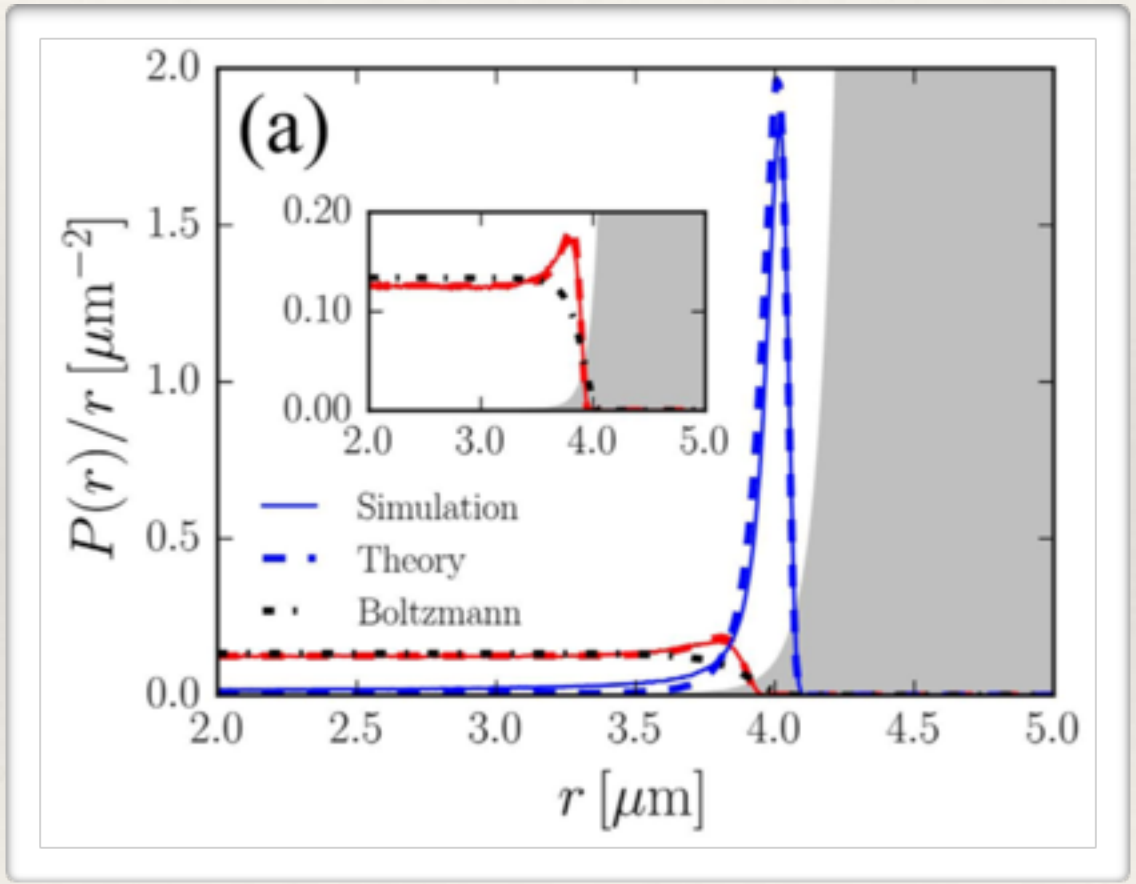
Generalizations to higher dimensions

UCNA

Two particles in 1D



Radial potential

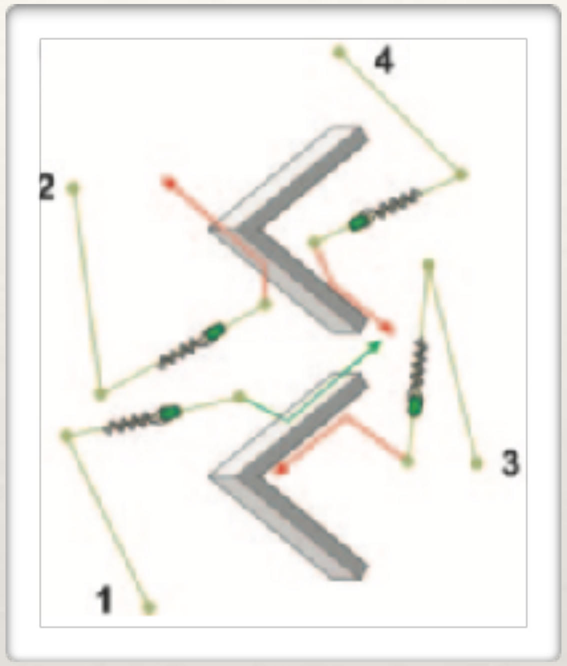


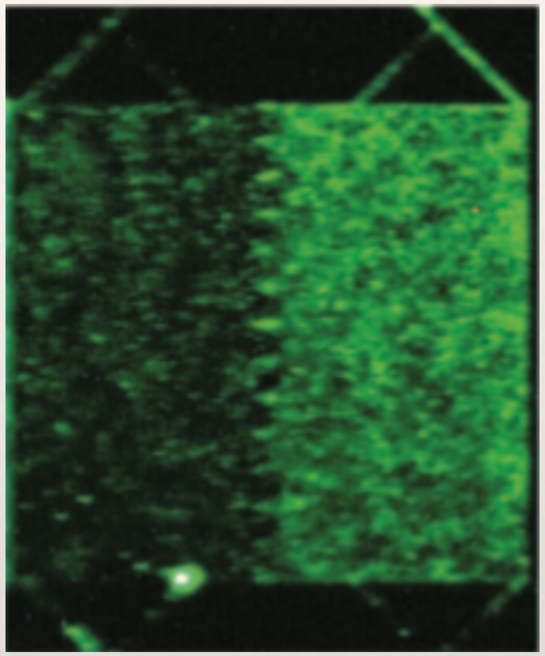
[Maggi *et al.*, Sci. Rep. **5**, 042601 (2015)], [Marconi & Maggi, Soft Matter **11**, 8768 (2015)]

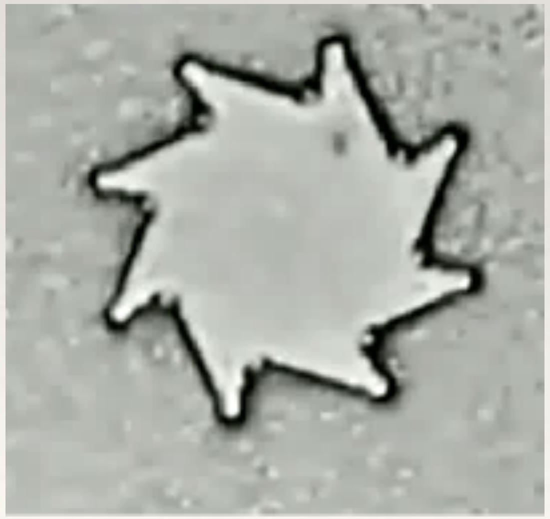
Density gradients & currents

- Asymmetric obstacles
  + Self-propelled particles
  $\Longrightarrow$ Rectified currents &
  Density gradients
- Micromotors

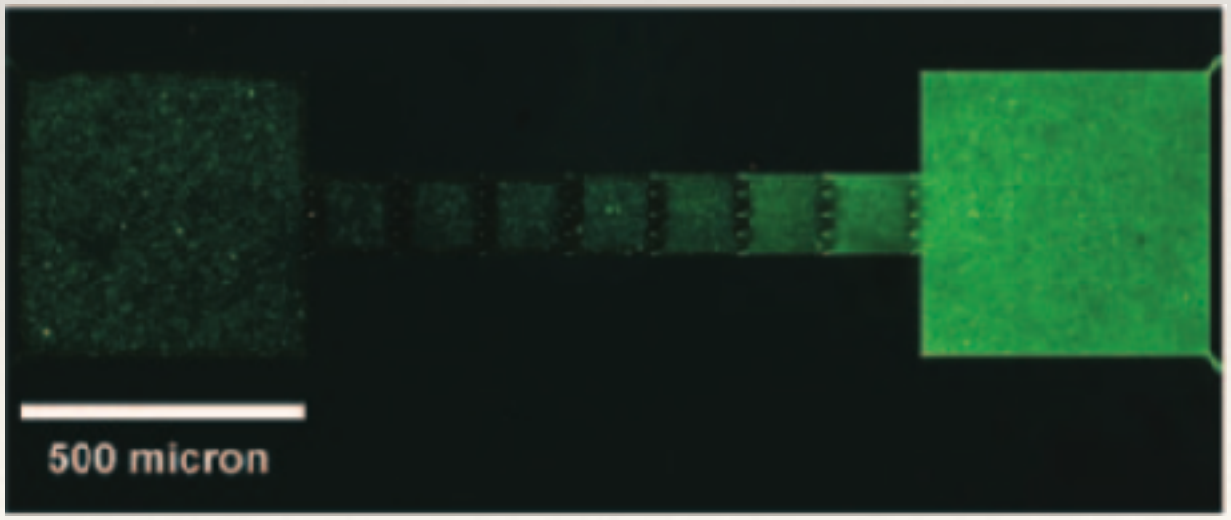
Density gradients of *E. coli*







E. coli-driven ratchet
[Di Leonardo *et. al.*, PNAS **107**, 9541 (2010)]



[Galajda *et. al.*, J. Bacteriol. **189**, 8704 (2007)]

But the UCNA can only yield equilibrium-like solutions.

Why do we fail to identify any rectified currents?

Artifact of the approximation? ~~Shortcoming of the model?~~

Need for a systematic small-τ expansion.

Small-τ expansion

$$\dot{\hat{x}} = -V'(\hat{x}) + \hat{v} \quad \Rightarrow \quad \partial_t\, \delta(\hat{x}(t) - x) = [\partial_x V' - \hat{v}\, \partial_x]\, \delta(\hat{x}(t) - x)$$

$$\equiv \hat{L}(t)$$

$$P(x,t) = \left\langle \mathcal{T} \mathrm{e}^{\int_0^t ds\, \hat{L}(s)} \right\rangle \delta(\hat{x}(0) - x_0)$$

Time-ordering operator

$$= \mathcal{T} \exp \left[\sum_{n=1}^{\infty} \frac{1}{n!} \left\langle \left[\int_0^t ds\, \hat{L}(s) \right]^n \right\rangle_c \right] \delta(\hat{x}(0) - x_0)$$

Time-ordered cumulants

n-th order contributes to $O(\tau^{n/2})$

Small-τ expansion

$$P(x,t) = \mathcal{T}\exp\left[\sum_{n=1}^{\infty}\frac{1}{n!}\left\langle\left[\int_0^t ds\,\hat{L}(s)\right]^n\right\rangle_c\right]\delta(\hat{x}(0)-x_0)$$

$$= \exp\left\{\int_0^t ds\,\left[M_0(s)+\tau M_1(s)+\tau^2 M_2(s)+\cdots\right]\right\}$$

M's can be calculated using the method of van Kampen, Physica **74**, 239 (1974)

$$\partial_t P = (M_0 + \tau M_1 + \tau^2 M_2 + \cdots)P$$

$$= \partial_x(V'P) + D\,\partial_x^2 P - \tau D\,\partial_x^2(V''P)$$

$$+\tau^2 D\left\{\partial_x^2\left[\left(V''^2 - V^{(3)}V' + DV^{(4)}\right)P\right] - \frac{3}{2}D\,\partial_x^3(V^{(3)}P)\right\} + O(\tau^3)$$

UCNA

$$\partial_t P = \partial_x \left(\frac{V'P}{1+\tau V''} \right) + D \left(\partial_x \, \frac{1}{1+\tau V''} \right)^2 P$$

Small-τ expansion

$$\partial_t P = \partial_x (V'P) + D\, \partial_x^2 P - \tau D\, \partial_x^2 (V''P)$$
$$+ \tau^2 D \left\{ \partial_x^2 \left[\left(V''^2 - V^{(3)} V' + D V^{(4)} \right) P \right] - \frac{3}{2} D\, \partial_x^3 (V^{(3)} P) \right\} + O(\tau^3)$$

- The UCNA is equivalent to the small-τ expansion only at the zeroth order.
- At first order, self-propulsion modifies the diffusion coefficient.
(may induce effective attraction if the potential is convex)
- Up to the second order, the effect of the Gaussian colored noise is equivalent to that of a non-Gaussian white noise with small but nonzero skewness.

NEQ steady state on a ring

- Current

Nonzero if the potential is asymmetric

$$J^{\mathrm{s}} = \frac{\tau^2}{2} \frac{\int_0^L dx\, V^{(3)} V'^2}{\int_0^L dx\, \mathrm{e}^{-V/D} \int_0^L dx\, \mathrm{e}^{V/D}} + O(\tau^3)$$

- Particle distribution

Generic long-range interactions mediated by active particles [YB et al. PRL (2018)]

$$P^{\mathrm{s}} \sim \exp\left\{ -\frac{V}{D} + \tau \left[V'' - \frac{V'^2}{2D} \right] + \tau^2 \left[\frac{DV^{(4)}}{2} - \frac{(V''^2 + 4V^{(3)}V')}{4} \right] + \frac{\tau^2}{D} \int_0^x dx' \left[\frac{V^{(3)}(x')V'(x')^2}{2} - \frac{J^{\mathrm{s}}}{Z_0} \mathrm{e}^{V(x')/D} \right] + O(\tau^3) \right\}$$

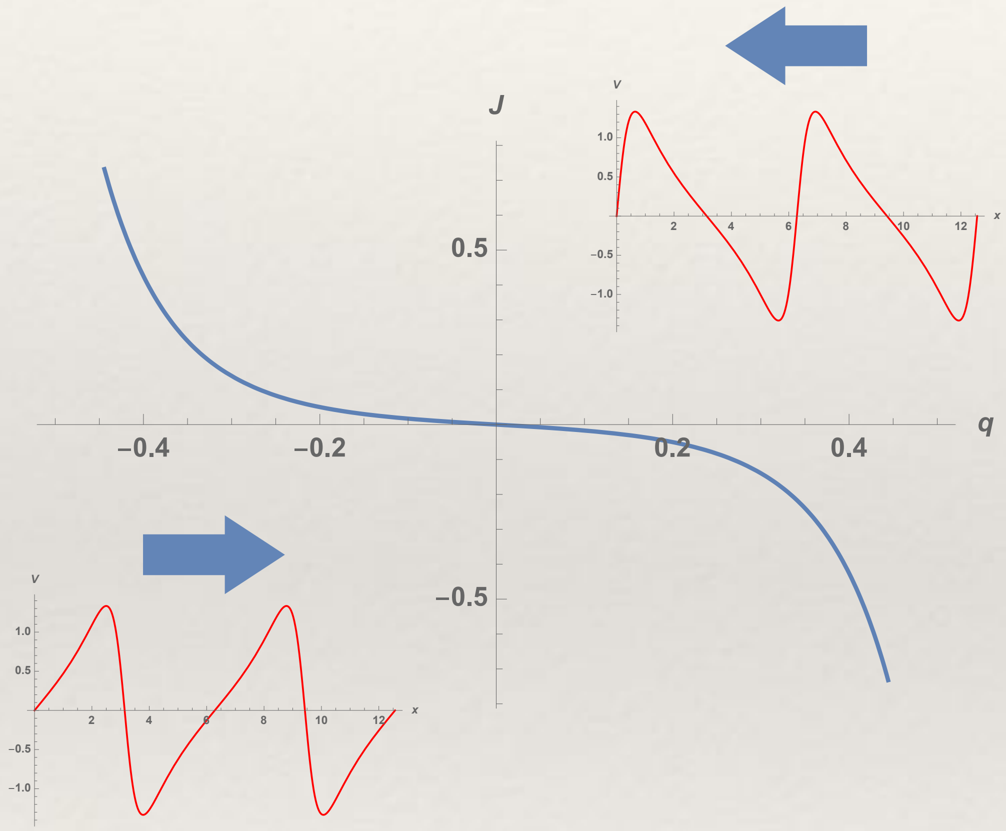
Agreement with the UCNA only up to first order

Nonlocal effects

$$Z_0 \equiv \int_0^L dx\, \mathrm{e}^{-V/D}$$

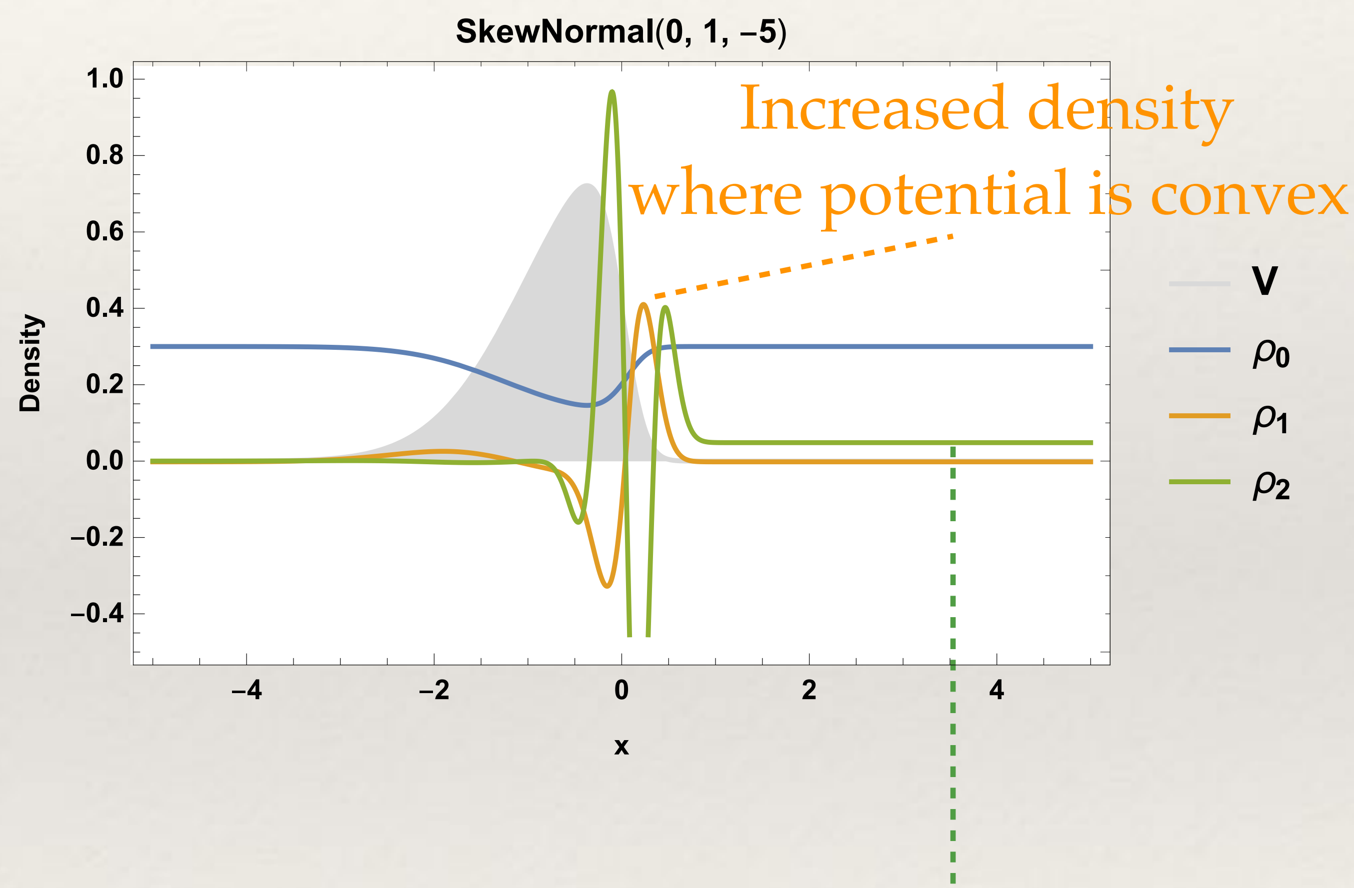
Steady-state current & density

1-d periodic ratchet potential



$$V_q(x) = \frac{\sin x}{1 + q^2 - 2q\cos x}$$

1-d skewed potential

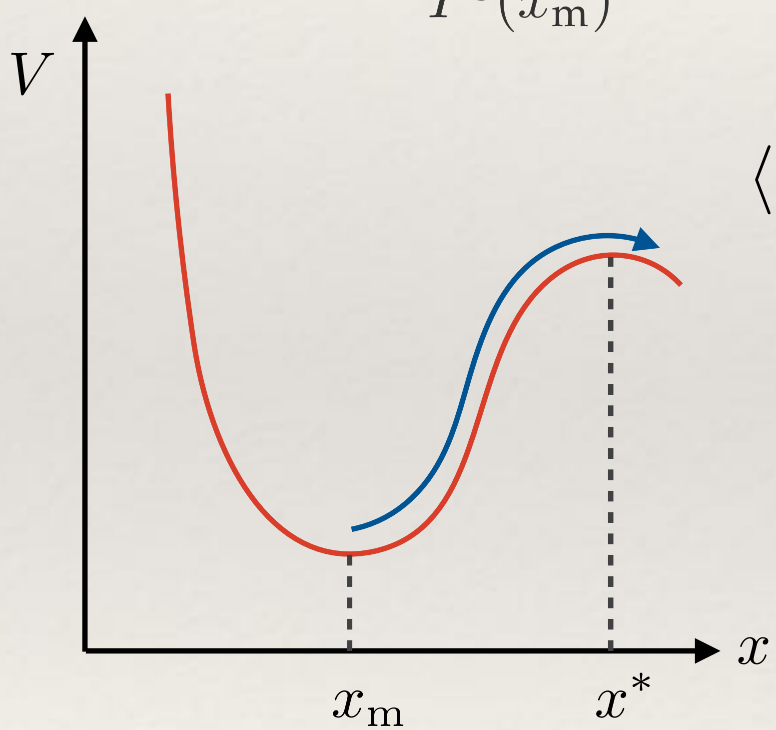


Second-order correction:
nonvanishing long-range effects

Modified Arrhenius Law

For small D,

Exit rate $\sim \dfrac{P^{\mathrm{s}}(x^*)}{P^{\mathrm{s}}(x_{\mathrm{m}})}$



Mean escape time:

Contributed by effective attraction

$$\langle t_{\mathrm{esc}} \rangle \sim \left\{ 1 + \frac{\tau}{2} \left[V''(x_{\mathrm{m}}) - V''(x^*) \right] + \frac{\tau^2}{8} \left[V''(x^*) - V''(x_{\mathrm{m}}) \right]^2 \right\}$$
$$\times \exp \left\{ \frac{1}{D} \left[V(x^*) - V(x_{\mathrm{m}}) - \frac{\tau^2}{2} \int_{x_{\mathrm{m}}}^{x^*} dx\, V^{(3)} (V')^2 \right] \right\}$$

Contributed by steady-state current
Requires non-Gaussian effects

Same result also obtained by calculations based on path integrals

Refs: [Bray, McKane, Newman, PRA (1990)] [Luckock, McKane, PRA (1990)]

Generalization to higher dimensions

$$\partial_t P = \partial_x (V' P) + D\,\partial_x^2 P - \tau D\,\partial_x^2 (V'' P) + \tau^2 D \left\{ \partial_x^2 \left[\left(V''^2 - V^{(3)} V' + D V^{(4)} \right) P \right] - \frac{3}{2} D\,\partial_x^3 (V^{(3)} P) \right\} + O(\tau^3)$$

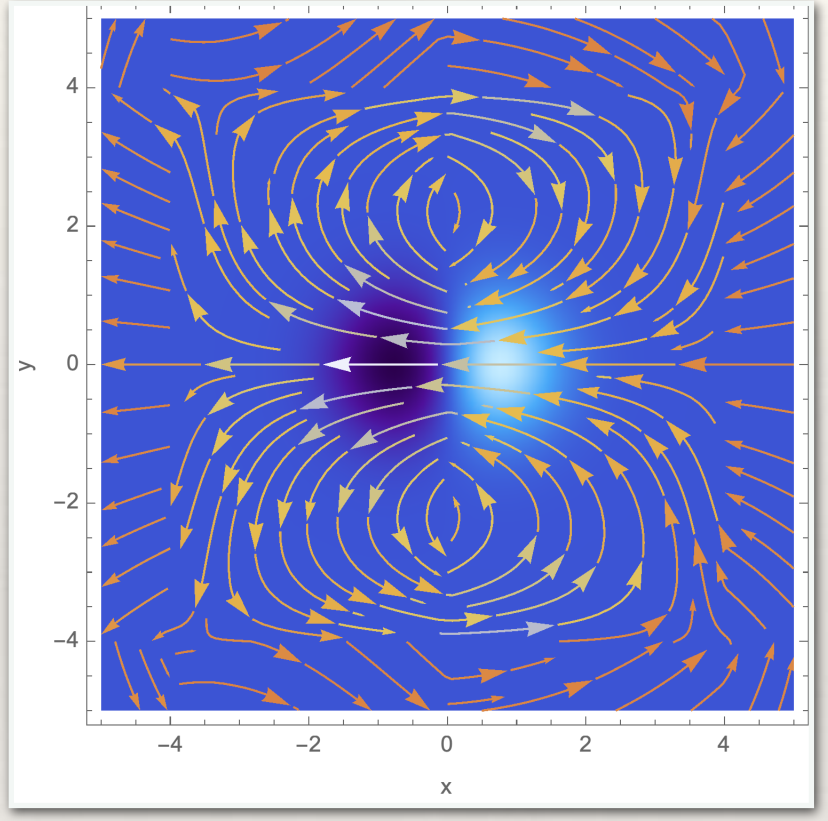
Change of effective diffusivity

$$\partial_t P = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} V) P + D \nabla^2 P - \tau D\, \boldsymbol{\nabla}\boldsymbol{\nabla} : (\boldsymbol{\nabla}\boldsymbol{\nabla} V) P + \tau^2 D \boldsymbol{\nabla}\boldsymbol{\nabla} : \left[(\boldsymbol{\nabla}\boldsymbol{\nabla} V) \cdot (\boldsymbol{\nabla}\boldsymbol{\nabla} V) - (\boldsymbol{\nabla}\boldsymbol{\nabla}\boldsymbol{\nabla} V) \cdot (\boldsymbol{\nabla} V) + D (\boldsymbol{\nabla}\boldsymbol{\nabla} \nabla^2 V) \right] P - \tau^2 \frac{3}{2} D^2\, \boldsymbol{\nabla}\boldsymbol{\nabla}\boldsymbol{\nabla} \,\vdots\, (\boldsymbol{\nabla}\boldsymbol{\nabla}\boldsymbol{\nabla} V) P + O(\tau^3)$$

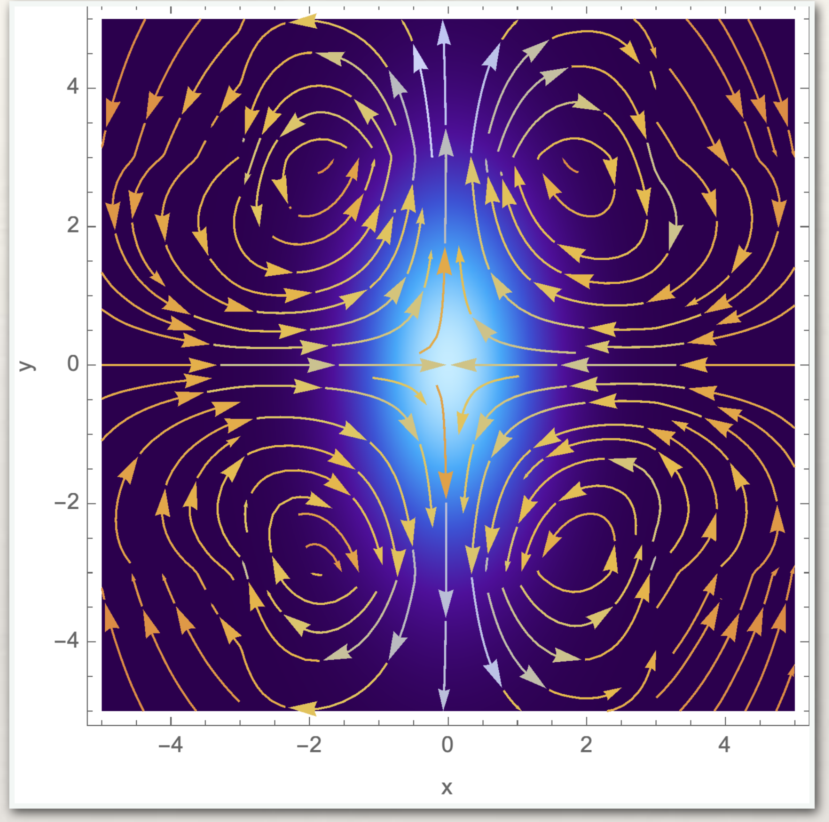
Non-Gaussian effects

Steady-state current on 2-d tori

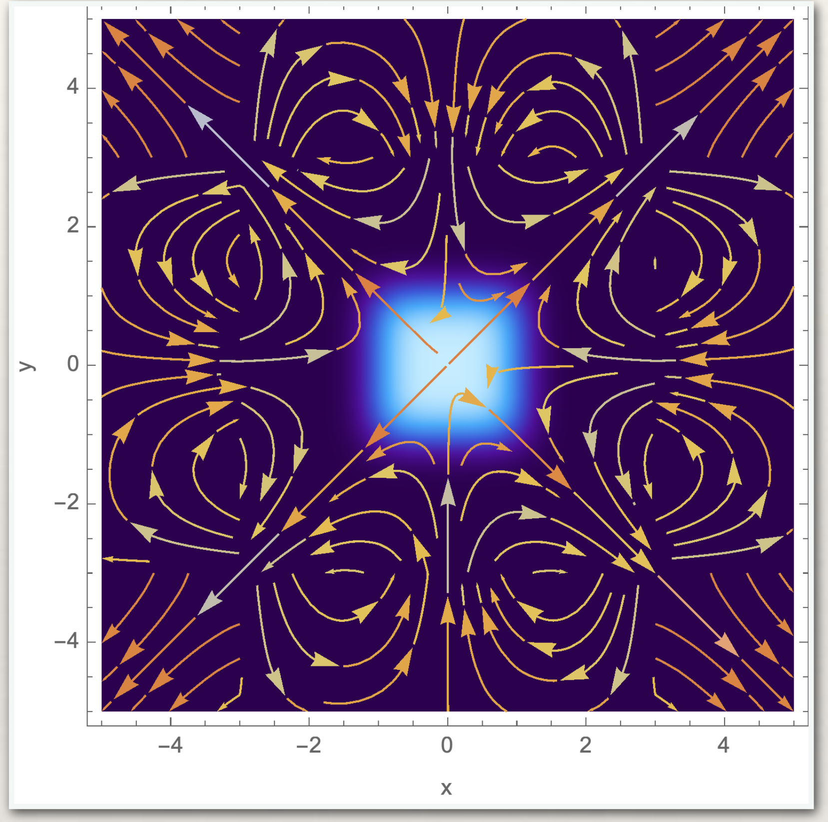
Asymmetric obstacle (dipole)



Elliptical obstacle (quadrupole)



Square obstacle (octopole)



- At second order, asymmetric objects behave like a multipole source generating long-range currents.

Bonus: Irreversibility

$$\hat{R}[x] \equiv \ln \frac{\mathcal{P}[x]}{\mathcal{P}[x^R]}$$

- Before Markovian approximation

$$\left\langle \frac{d\hat{R}}{dt} \right\rangle_{\mathrm{NM}}^{\mathrm{s}} = \frac{D\tau^2}{2} \int dx \, \frac{\mathrm{e}^{-V(x)/D}}{Z_0} V^{(3)}(x)^2 + O(\tau^3)$$

- After Markovian approximation

$$\left\langle \frac{d\hat{R}}{dt} \right\rangle_{\mathrm{M}}^{\mathrm{s}} = \frac{9D\tau^2}{8} \int dx \, \frac{\mathrm{e}^{-V(x)/D}}{Z_0} V^{(3)}(x)^2 + O(\tau^3)$$

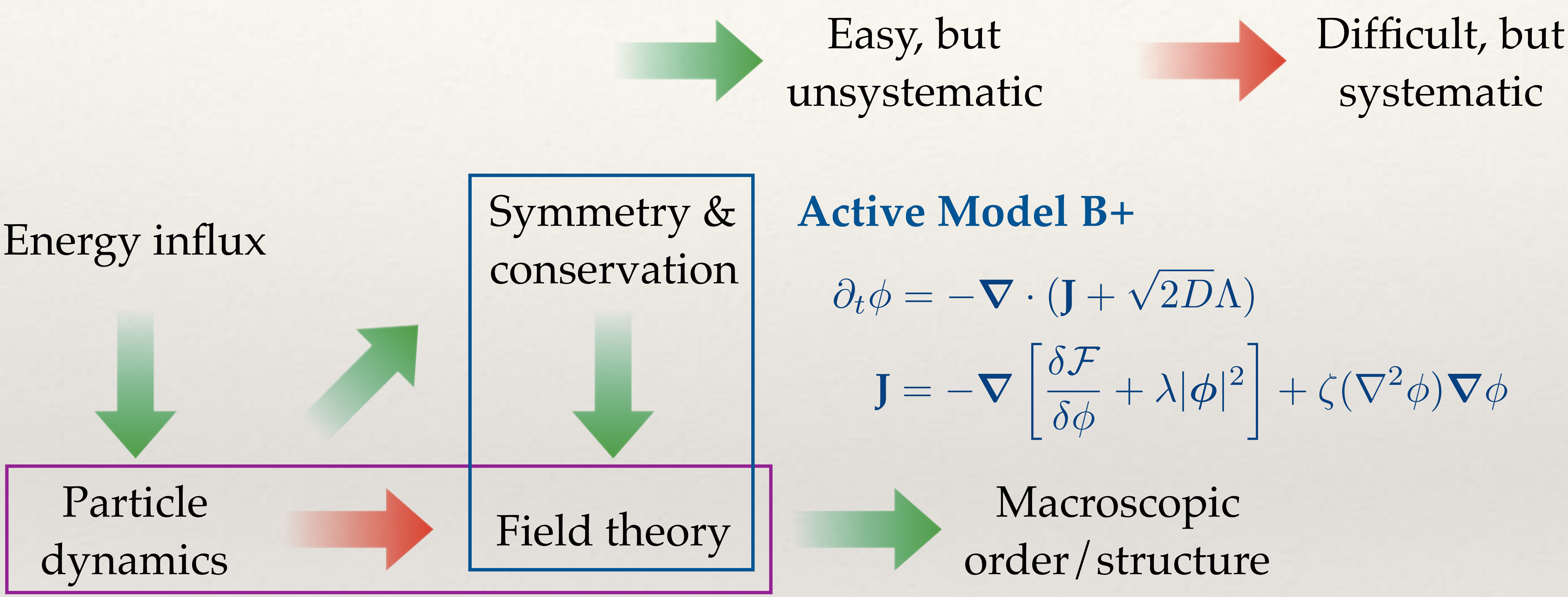
$$\left\langle \frac{d\hat{R}}{dt} \right\rangle_{\mathrm{M}}^{\mathrm{s}} > \left\langle \frac{d\hat{R}}{dt} \right\rangle_{\mathrm{NM}}^{\mathrm{s}}$$

Negative "hidden entropy" production!

Summary

- The UCNA correctly captures the first-order effects of colored noise in the steady state but is unreliable for higher-order properties.
- A systematic small-τ expansion shows that, up to second order, the Gaussian colored noise is equivalent to the non-Gaussian white noise with nonzero skewness.
- The phase separation is described by an effective attraction at first order (EQ-like regime).
- Second-order corrections (non-Gaussian noise) are crucial for describing rectified currents and long-range effects.

Implication for active field theory



Active Model B+

$$\partial_t \phi = -\boldsymbol{\nabla} \cdot (\mathbf{J} + \sqrt{2D}\Lambda)$$

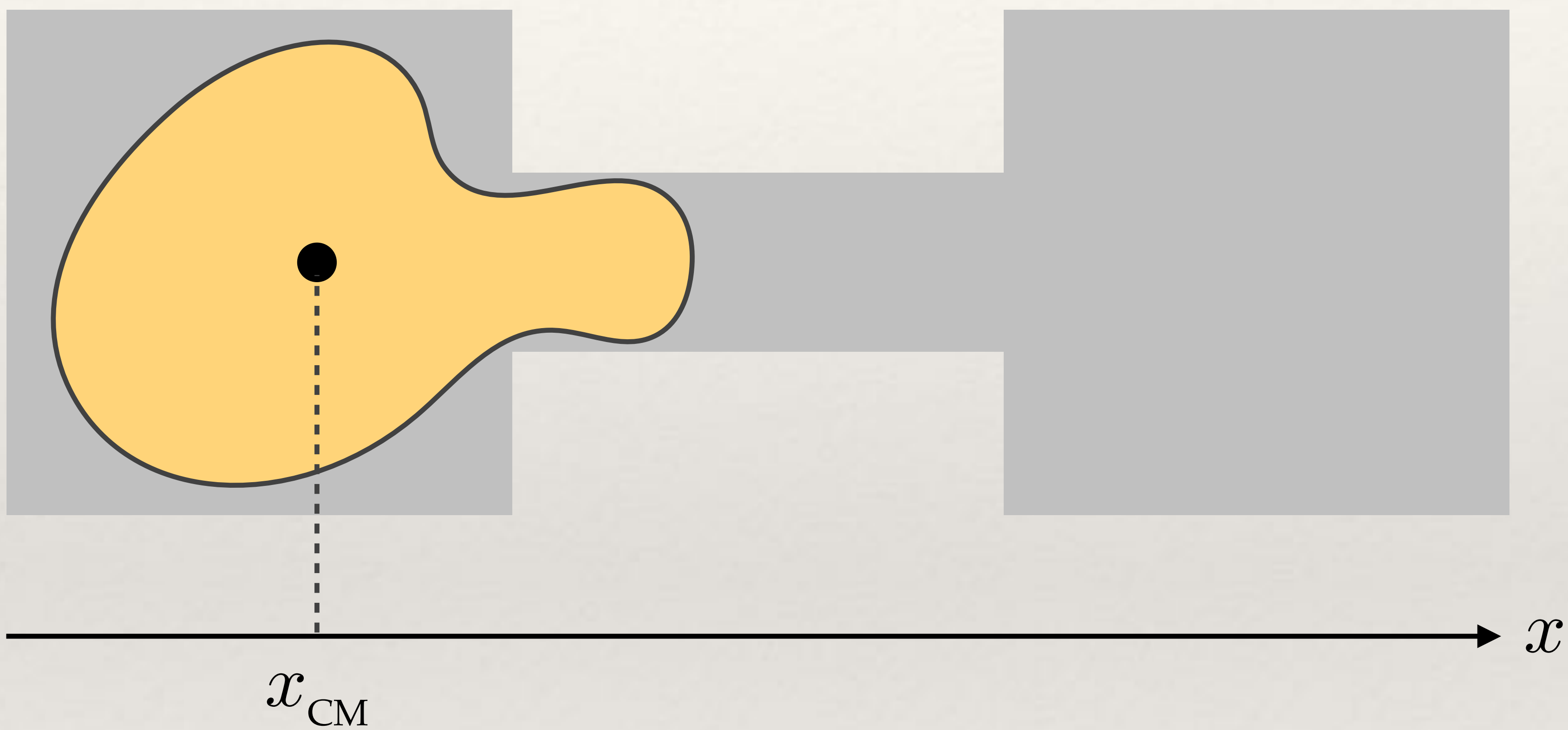
$$\mathbf{J} = -\boldsymbol{\nabla}\left[\frac{\delta \mathcal{F}}{\delta \phi} + \lambda |\boldsymbol{\phi}|^2\right] + \zeta(\nabla^2\phi)\boldsymbol{\nabla}\phi$$

A field theory with non-Gaussian noise determined by particle interactions?

cf. Case of constant noise cumulants:
[Fodor, Hayakawa, Tailleur, van Wijland, PRE (2018)]

Application to empirical models

Confined cell dynamics



$$\dot{x}_{\text{CM}} = -V'_{\text{eff}}(x_{\text{CM}}) + \xi \qquad \langle \xi(t)\xi(t') \rangle = \frac{D}{\tau} \mathrm{e}^{-t/\tau}$$

Deformation time scale

$$\langle \Delta x_{\text{CM}} \rangle \simeq -V'_{\text{eff}}(x_{\text{CM}})\Delta t \qquad \langle \Delta x^2_{\text{CM}} \rangle \simeq 2D\Delta t \qquad \boxed{\langle \Delta x^3_{\text{CM}} \rangle \simeq 9D\tau^2\, V^{(3)}_{\text{eff}}(x_{\text{CM}})\, \Delta t}$$

Extra time scale can be estimated by examining the third cumulant