Novel Features of Direction Reversing Active Brownian motion

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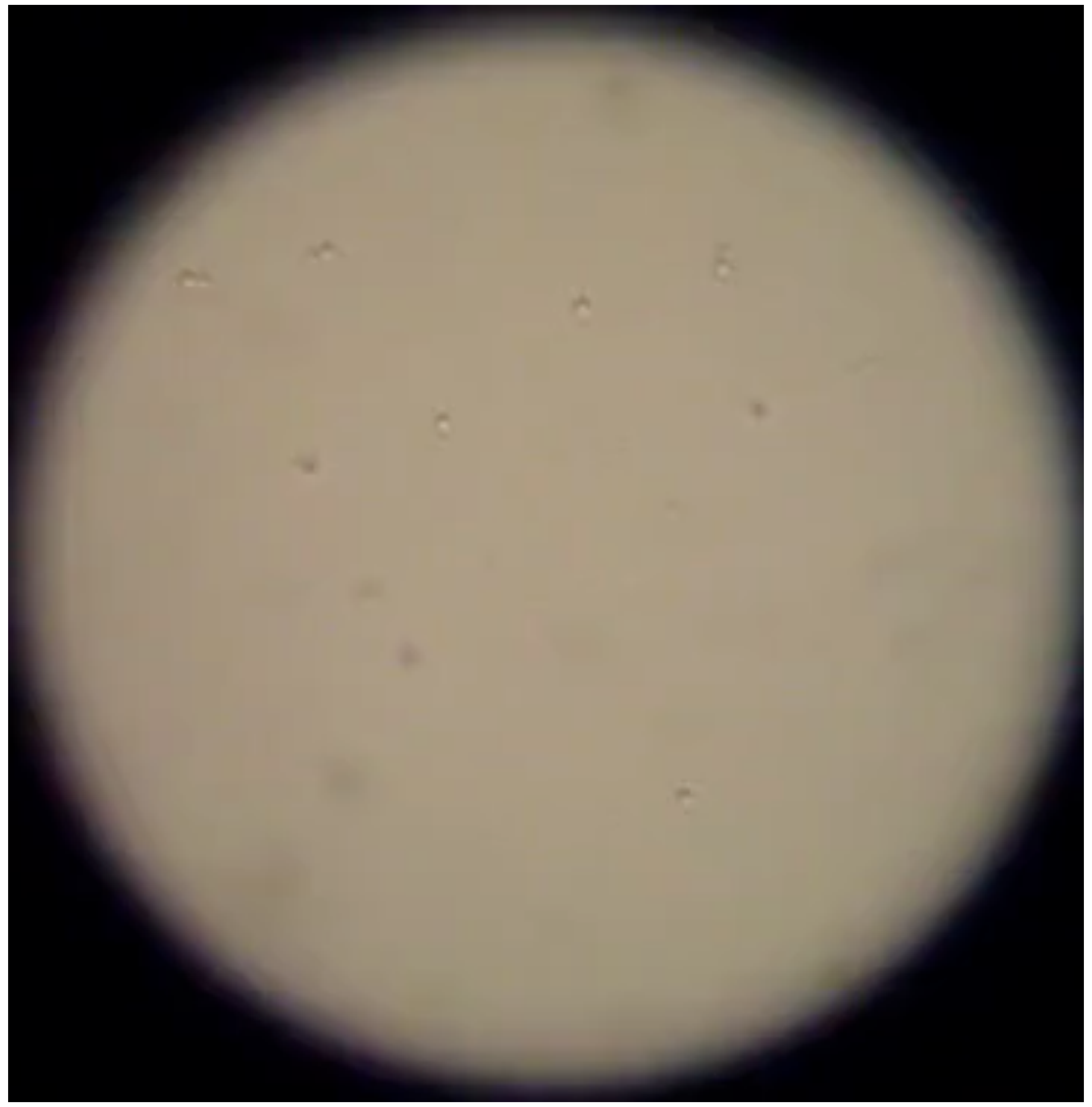
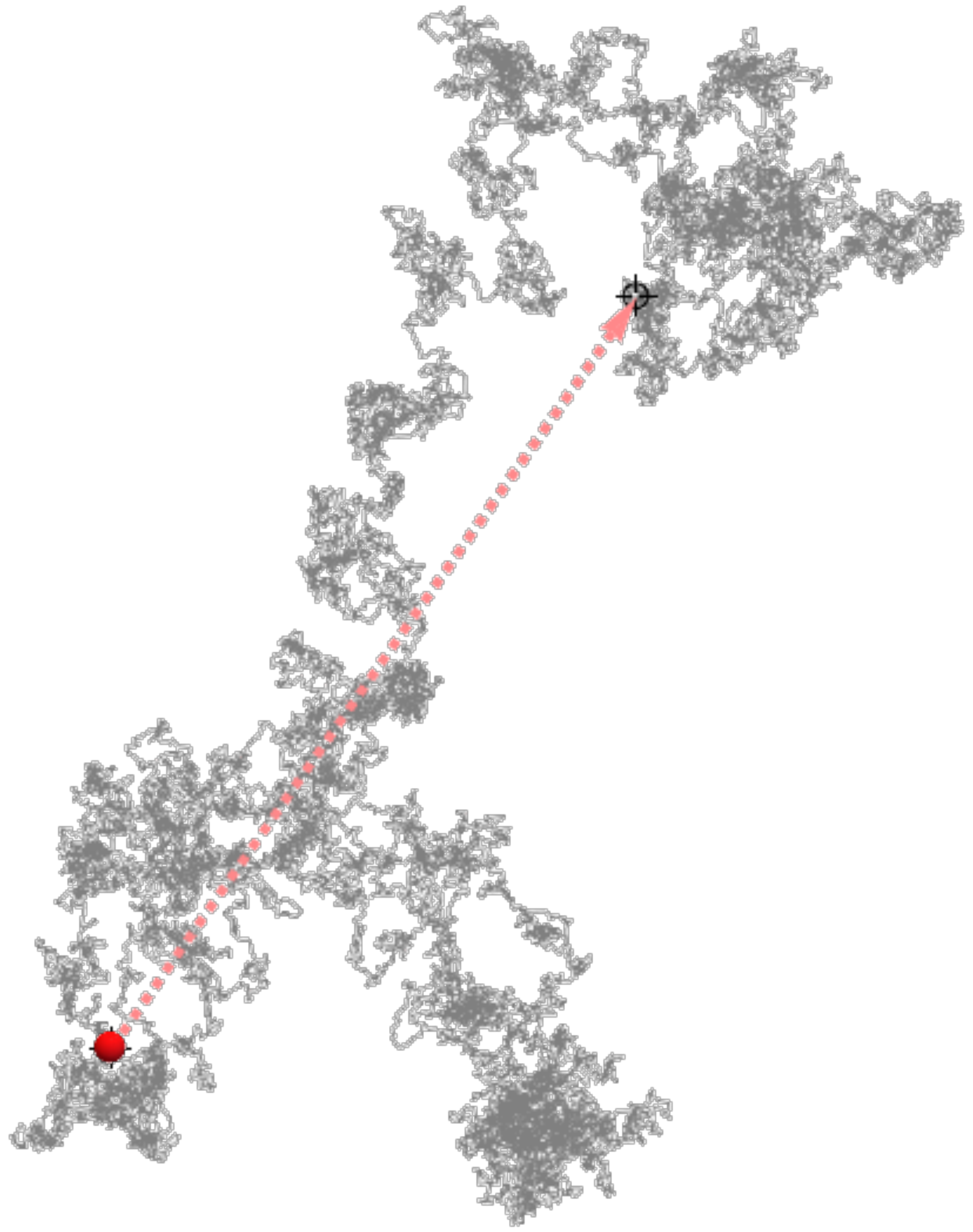
1. Phys. Rev. E **104**, L012601 (2021). [**Letter**]
2. Soft Matter **17**, 10108 (2021).

(also see the poster by Ion Santra)

Passive particle (Brownian motion)

The jittery motion of colloidal particles in water.





For a 1 μm silica bead in the water at room temperature, the viscous relaxation time $(m/\gamma) \sim$ 10–100 ns.

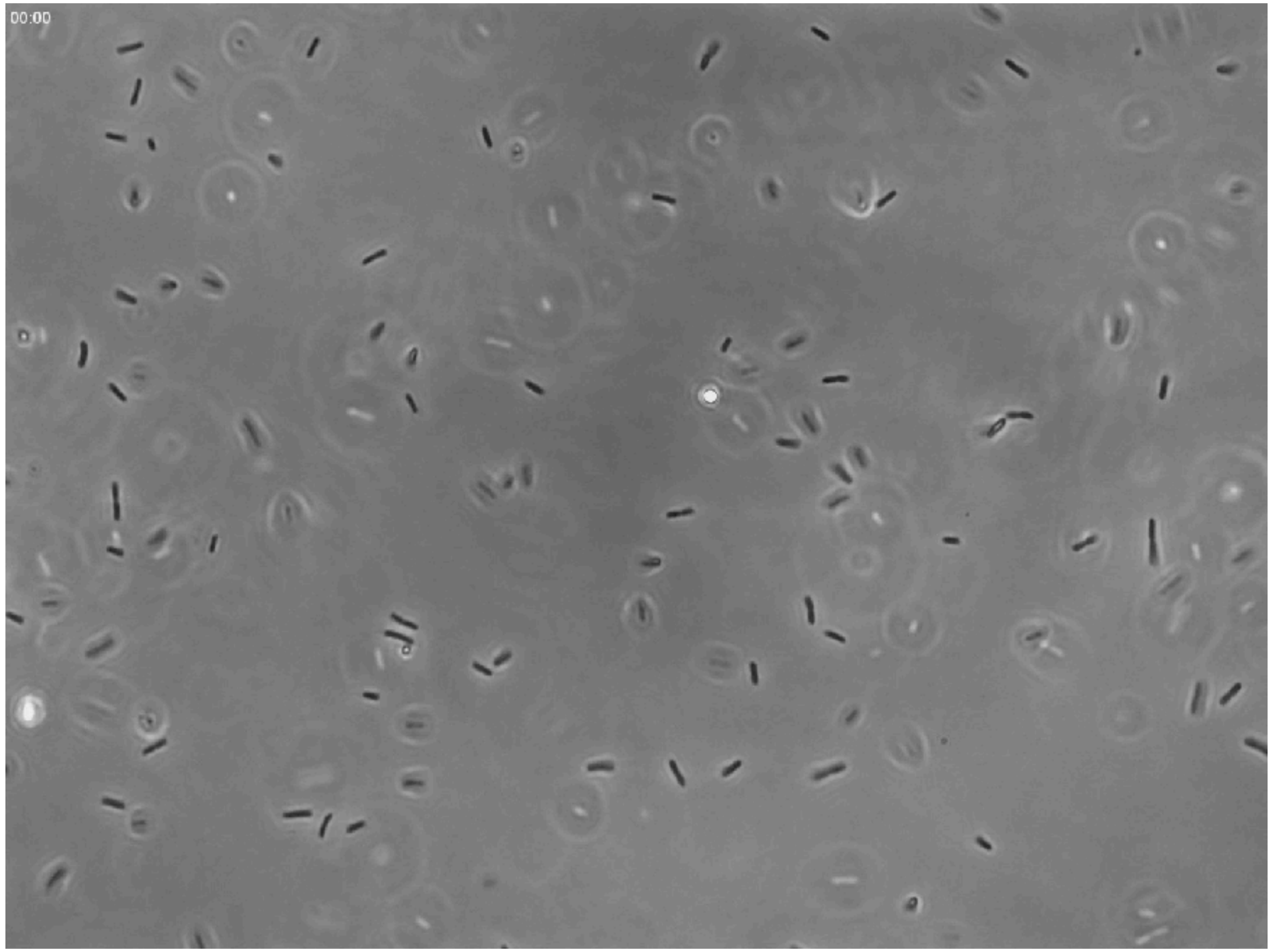
***Overdamped motion*— in a small time interval $\Delta t \gg (m/\gamma)$, the displacement along each direction is independently given by**

$$\Delta x_i = \sqrt{2D\Delta t}\,\xi_i$$

where $D = \frac{k_B T}{\gamma}$ and $p(\xi_i) = \frac{1}{\sqrt{2\pi}} e^{-\xi_i^2/2}$

For a 1 μm silica bead in the water at room temperature, $D \sim 0.1\,(\mu\text{m})^2/\text{s} \implies \Delta x \sim 1\,\mu$m for $\Delta t = 1$s [~ 1 nm in $1\mu s$]

Bacterial motion



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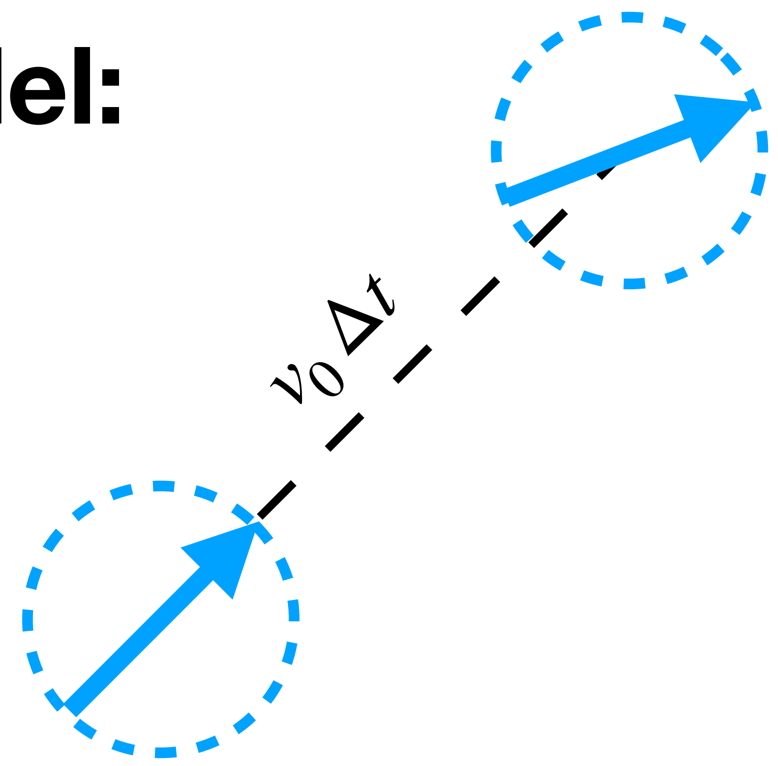
A bacterium self-propels itself with almost a constant speed along a stochastically evolving "internal direction".

An *E. coli*—a rod shaped bacterium of 1-2 μm long and about 1 μm in diameter —roughly moves with a speed of 30 μm/s.

Minimal theoretical model:

$$\Delta \vec{r} = v_0 \, \Delta t \, \hat{n} + \sqrt{2D\Delta t} \, \vec{\xi}$$



This persistent motion is referred to as active motion.

The unit vector $\hat{n}$ evolve stochastically.

Basic models of active motion

Run and tumble particle (RTP)

$\hat{n}$ changes by a finite amount
via an intermittent tumbling

Active Brownian particle (ABP)

$\hat{n}$ undergoes rotational diffusion

Two dimensions: $\hat{n} = (\cos\theta, \sin\theta)$

In a small time interval Δt

- **With probability $\gamma \Delta t$**

  $\theta \to \theta' \in (0,2\pi)$ uniformly

- **With probability $(1 - \gamma \Delta t)$**

  $\Delta x = (v_0 \cos\theta)\, \Delta t$

  $\Delta y = (v_0 \sin\theta)\, \Delta t$

$\Delta x = (v_0 \cos\theta)\, \Delta t$

$\Delta y = (v_0 \sin\theta)\, \Delta t$

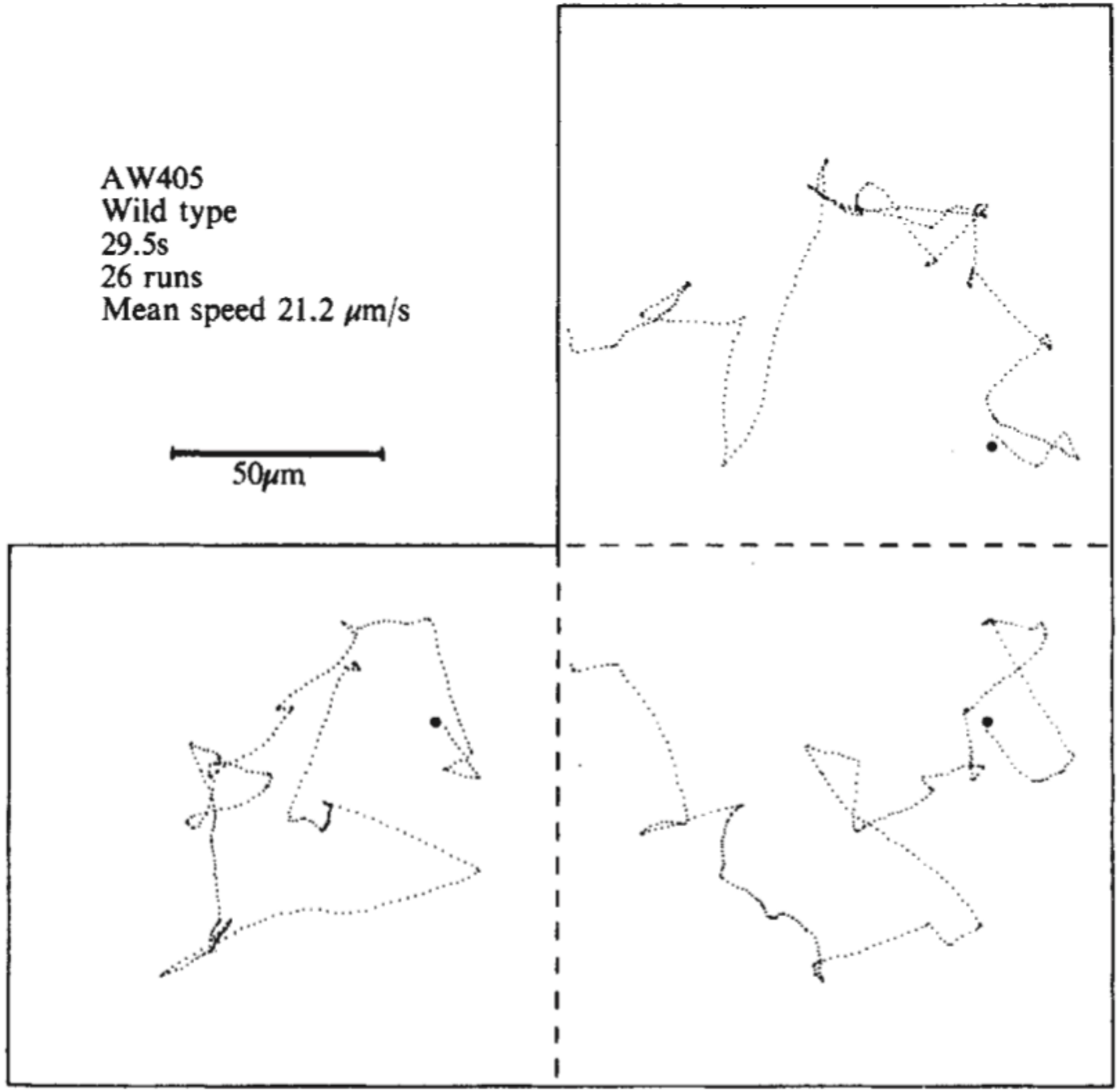
$\Delta\theta = \sqrt{2 D_{\mathrm{R}} \Delta t}\, \xi_\theta$

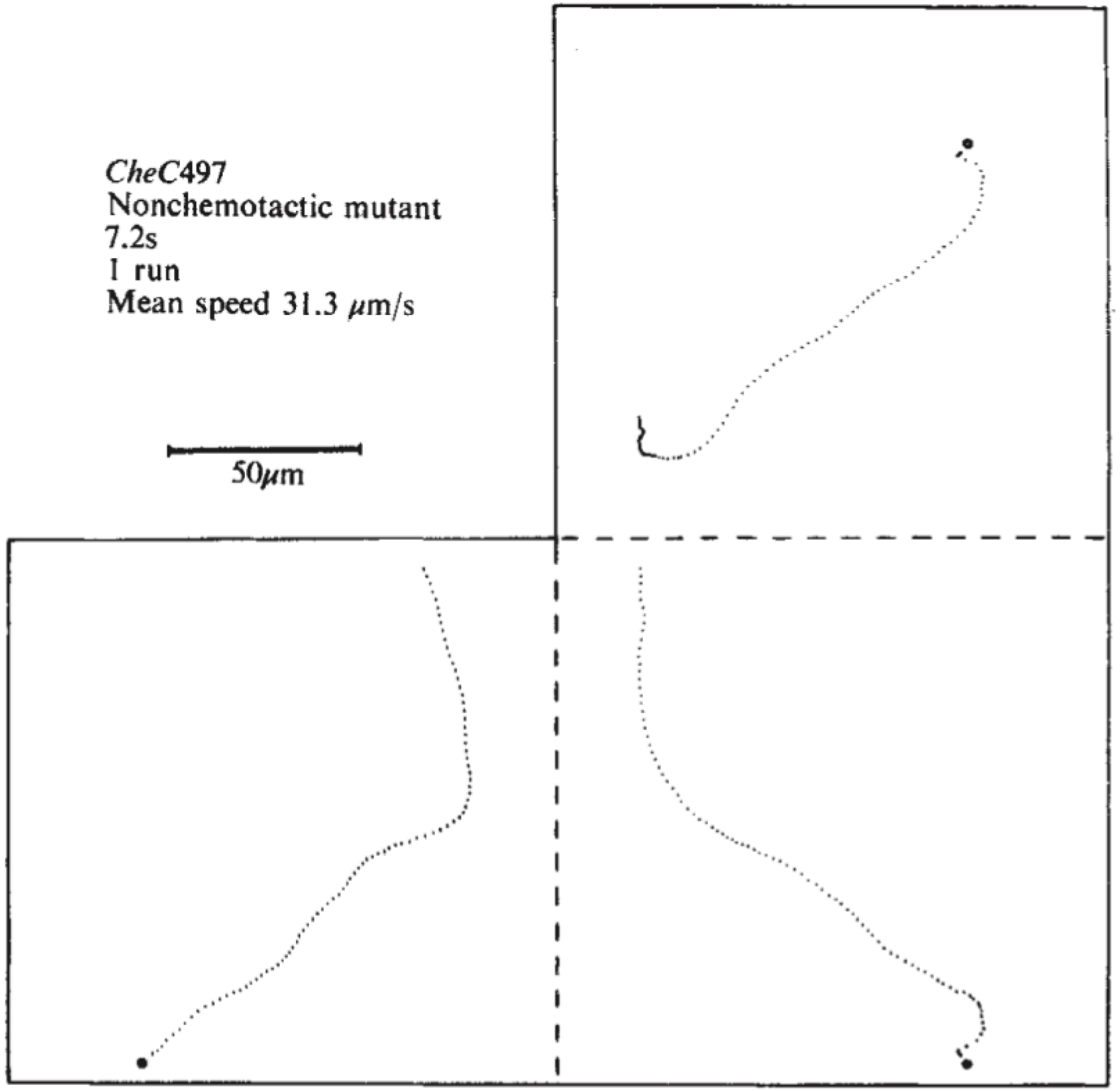
$$P(\xi_\theta) = \frac{e^{-\frac{1}{2}\xi_\theta^2}}{\sqrt{2\pi}}$$

These models successfully describe dynamics of bacteria like *E. coli.*

and some other artificial micro swimmers (Janus particles)

H. C. Berg & D. A. Brown

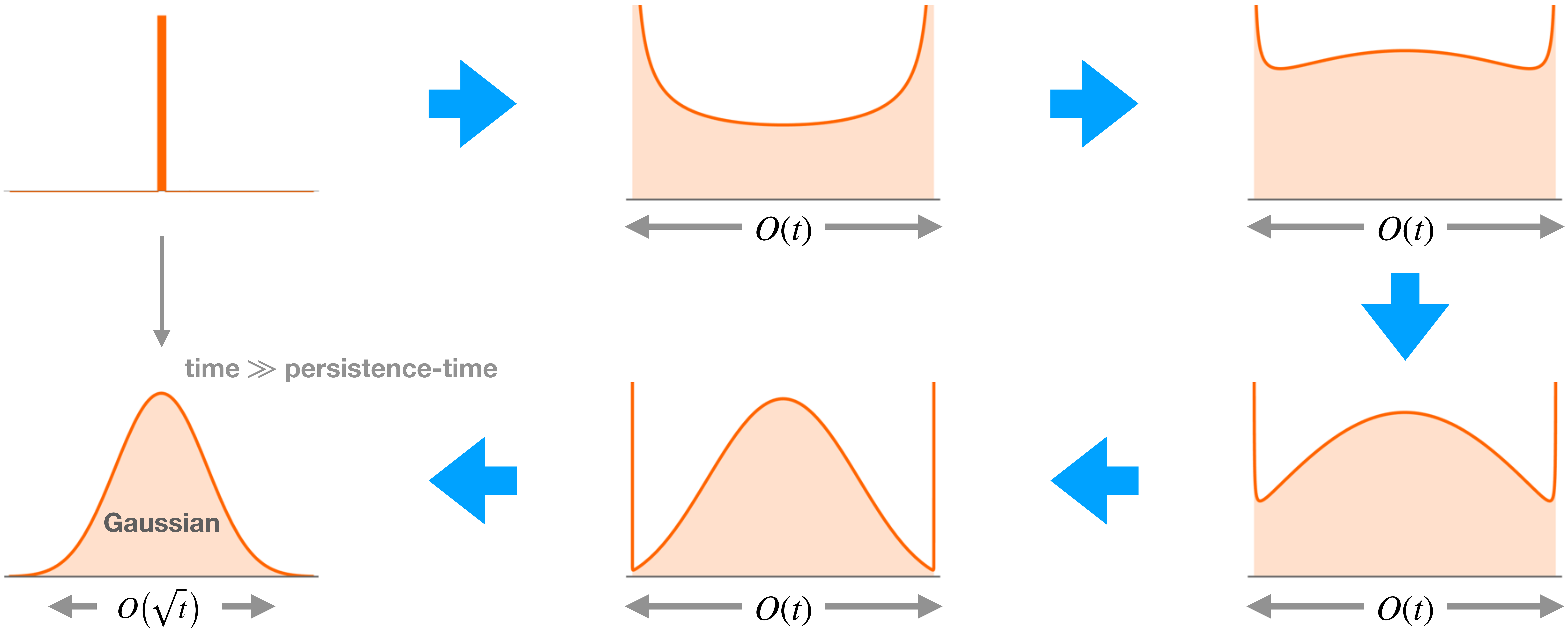




Generic features

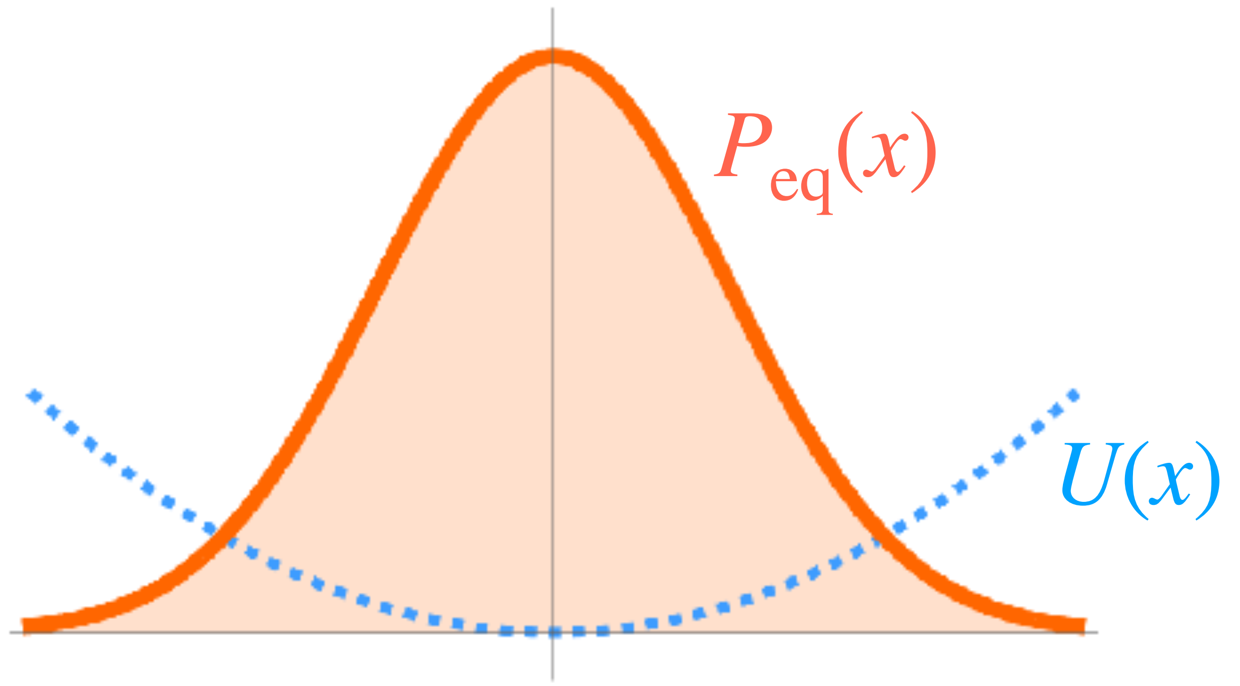
Generic features of position distribution

(As time progresses)



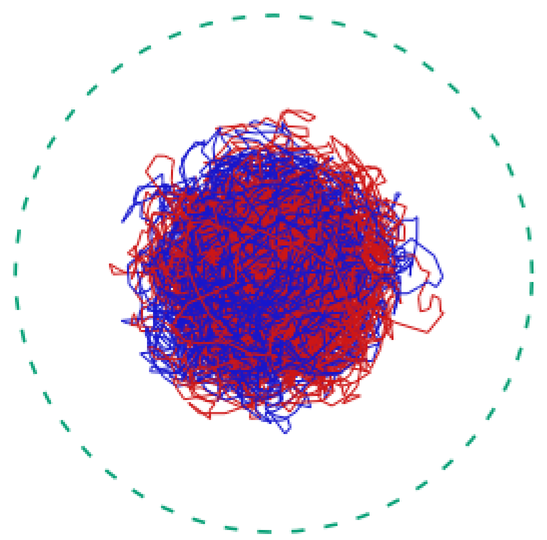
Stationary State in confinement

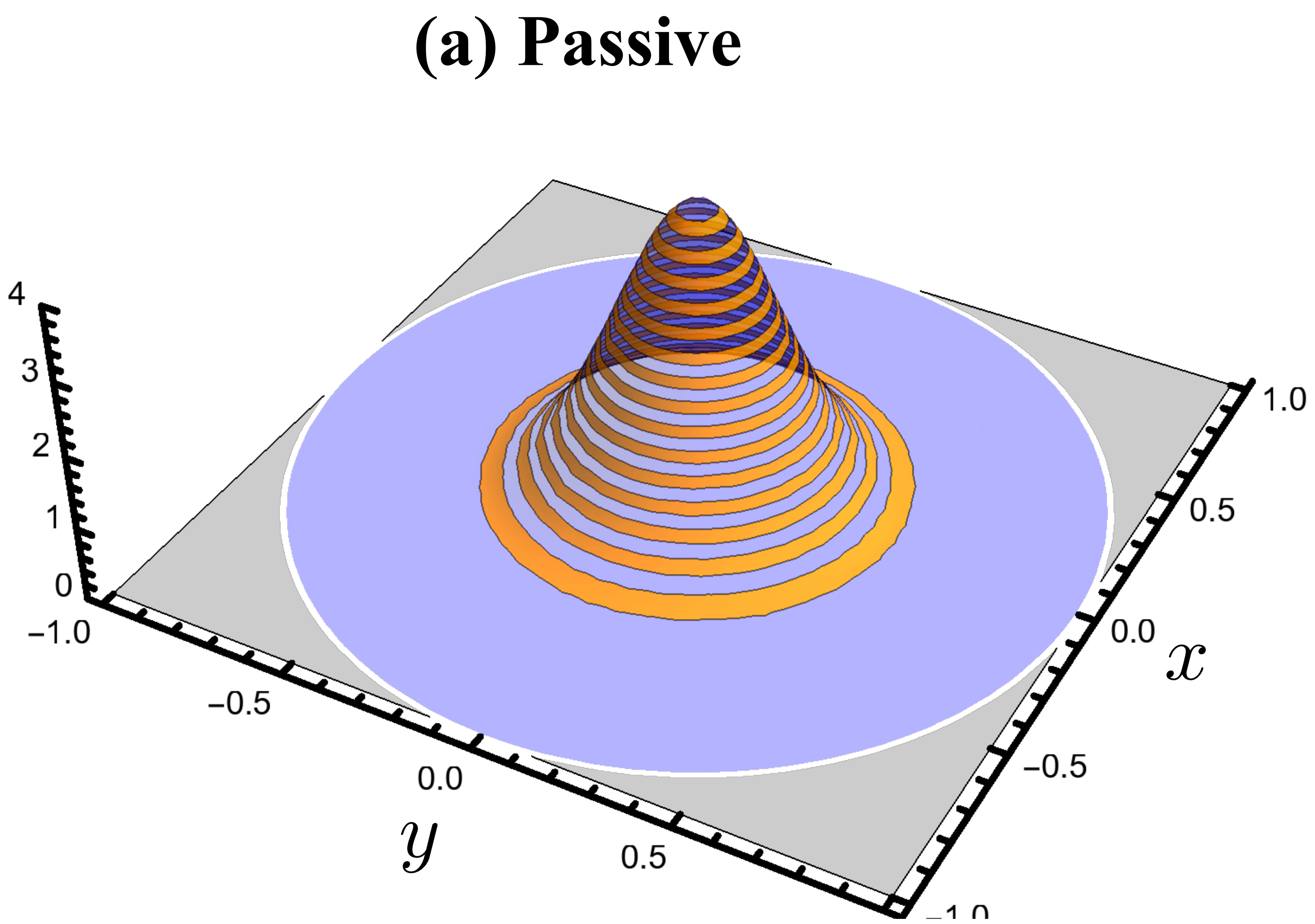
Passive (Brownian) particle: $P_{\mathrm{eq}}(x) = \dfrac{e^{-\beta U(x)}}{Z}$

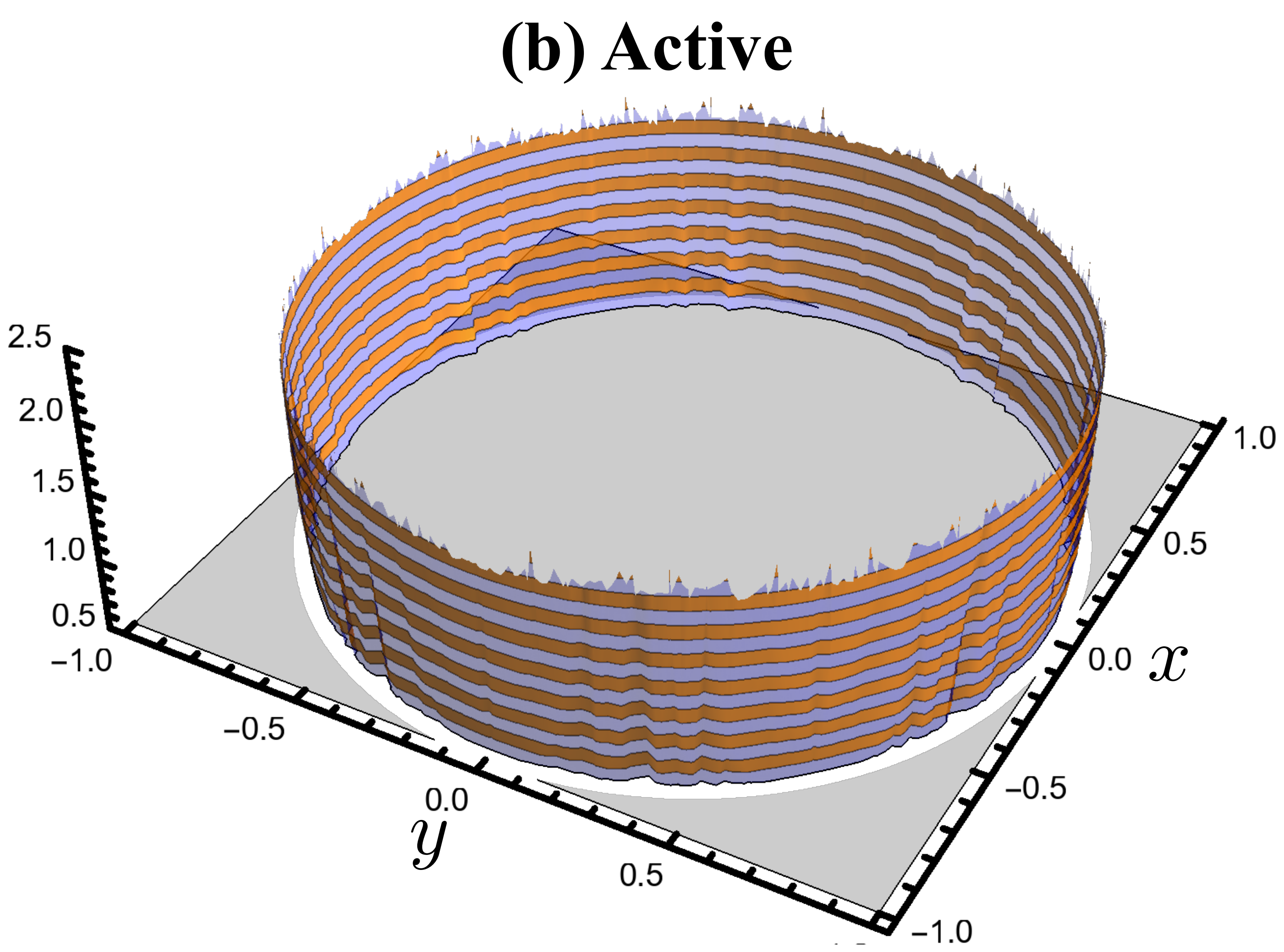


Active particle: generically two phases

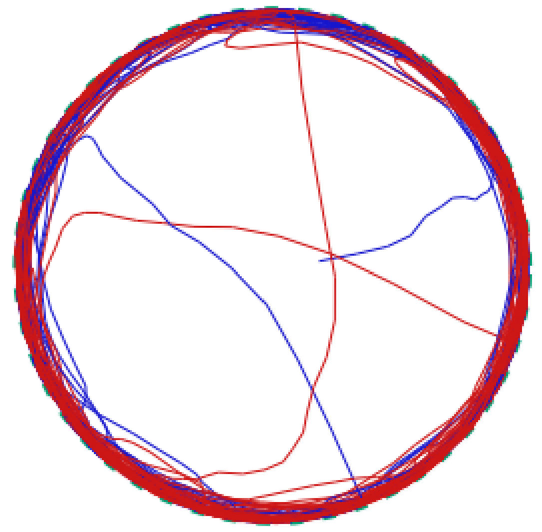
Persistence-time
≪ Relaxation-time





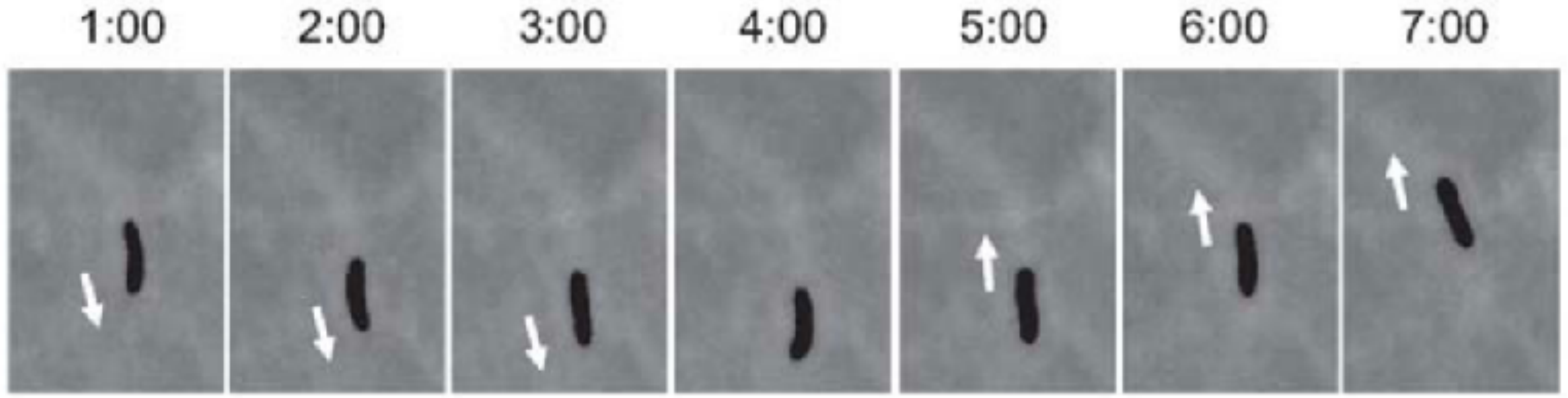


Persistence-time
≫ Relaxation-time



Active motion with two time scales

Direction reversing bacterial motion

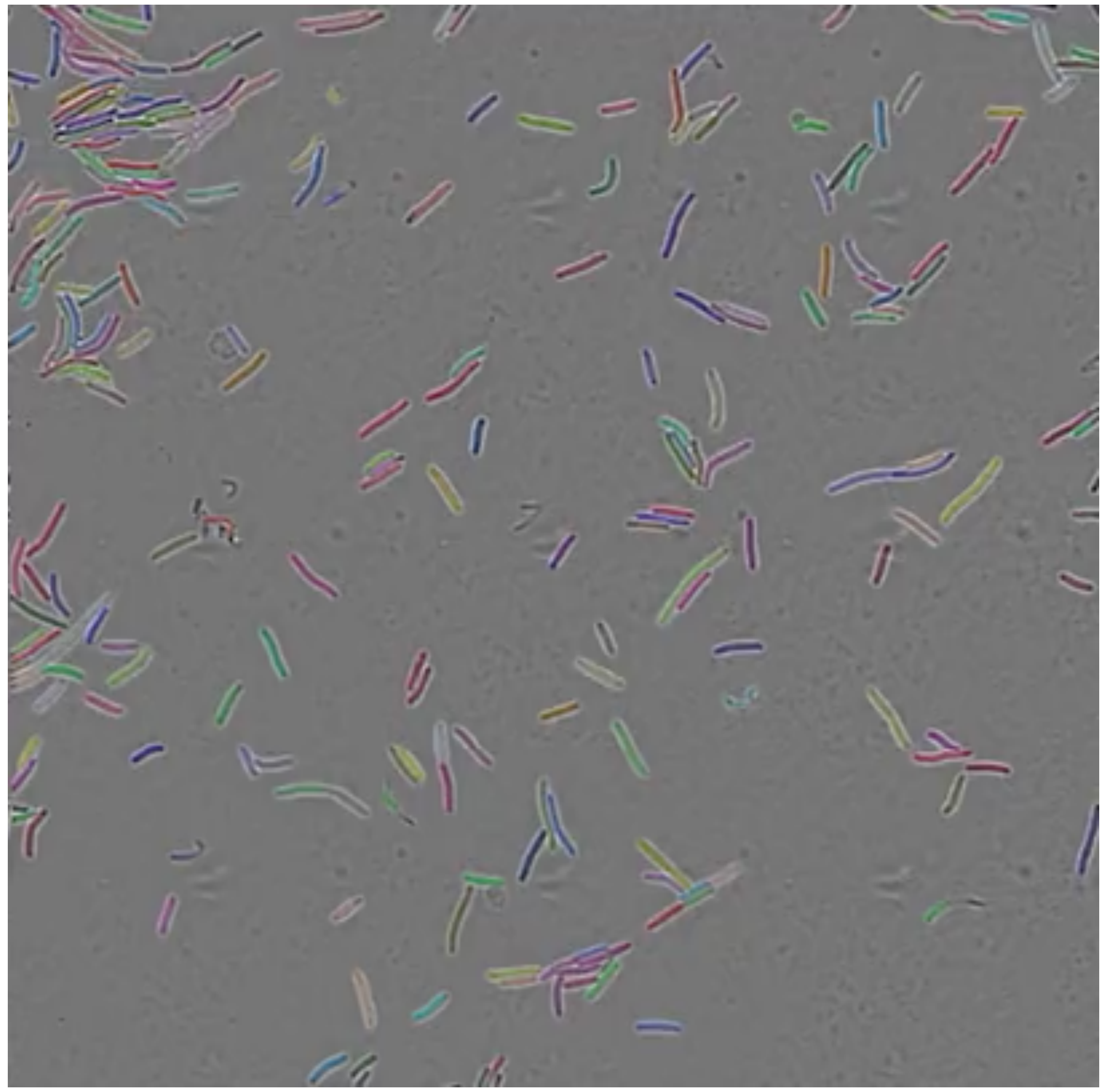


[Mol. BioSyst. 4, 1009 (2008)]

Myxococcus xanthus

Size $\sim 10 \times$ ***E. coli***

$v_0 \sim 1\mu$**m/min**



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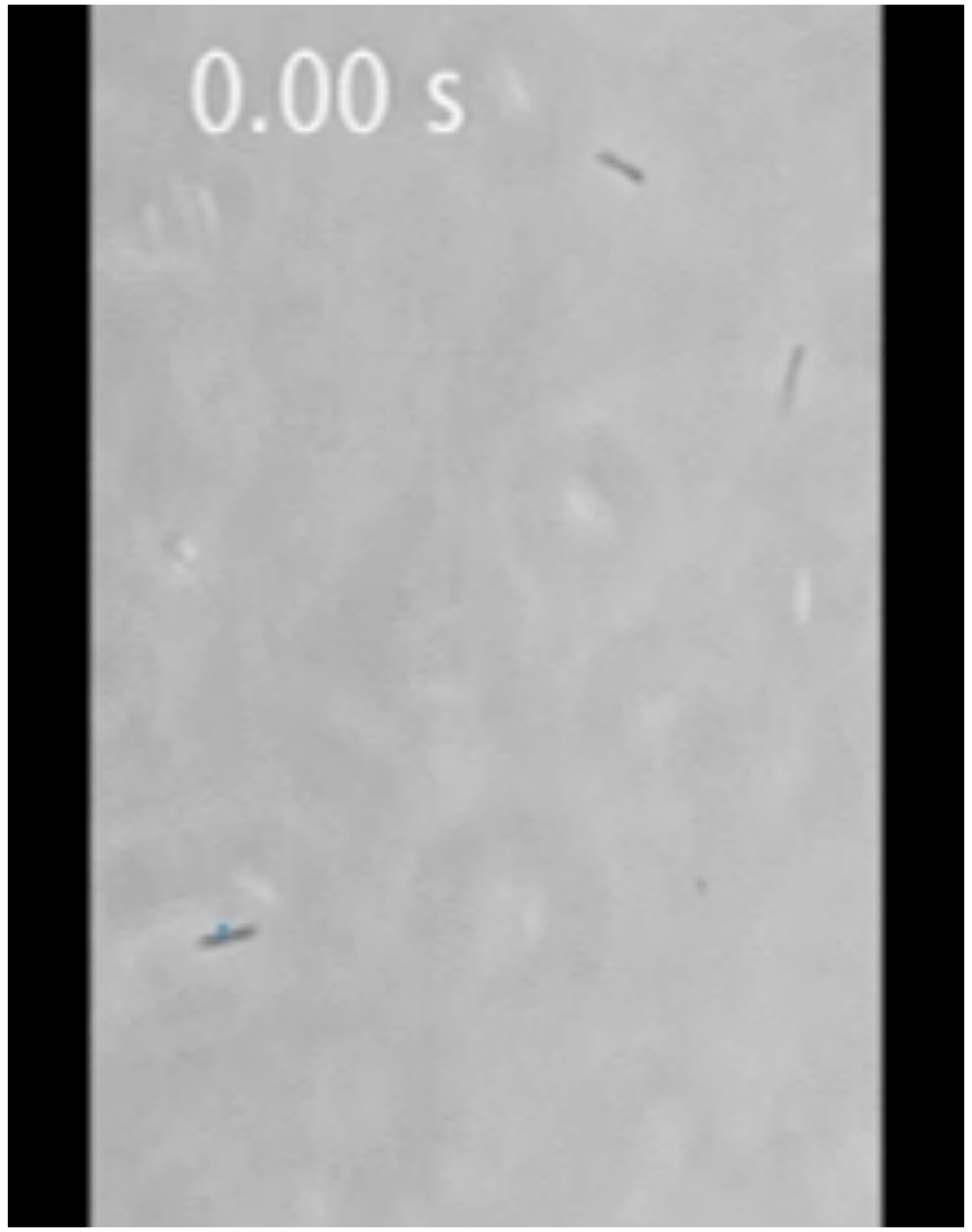
Other bacteria:

- ***Pseudoalteromonas haloplanktis***
- ***Shewanella putrefaciens***



[Biophys J. **105**, 1915 (2013)]

Pseudomonas putida

Size $\sim$ 2 μm × 5 μm

$v_0 \sim 20, 40\,(\rightarrow, \leftarrow)\,\mu$m/s

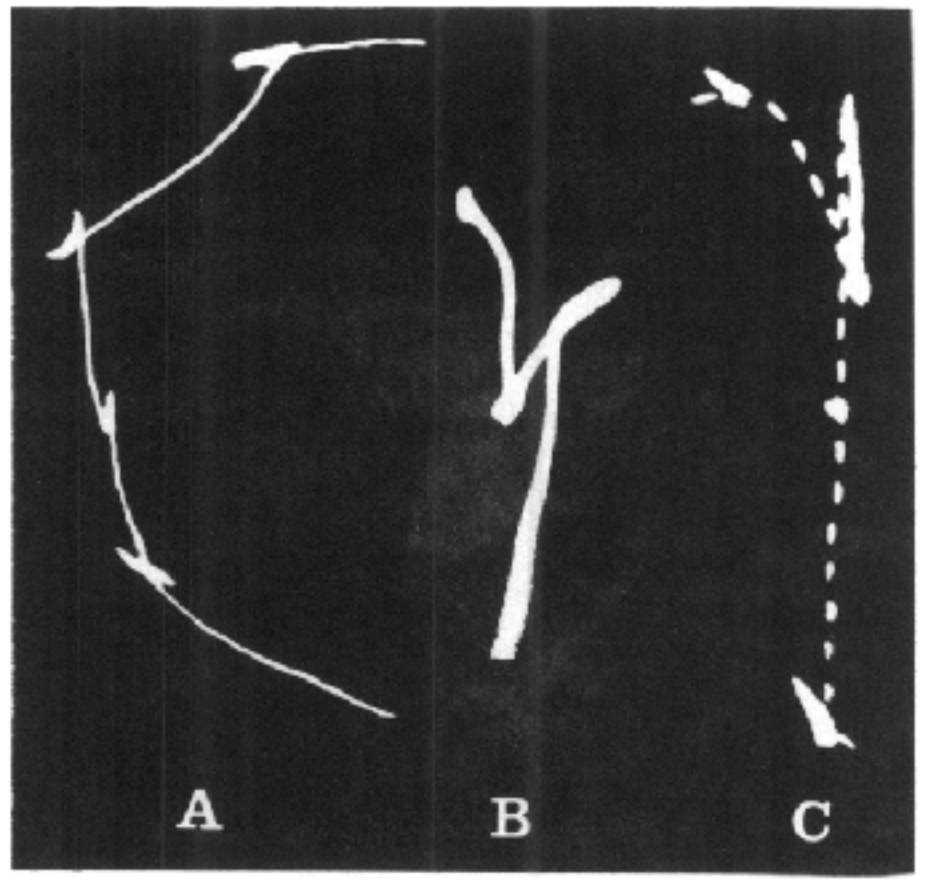


FIG. 1. *Motility tracks of Pseudomonas citronellolis. Photomicrographs were taken in dark field with a stroboscopic lamp operating at 60 (A and B) or 10 pulses per s (C). (A) The bacterium entered at the lower right and backed up four times during the exposure. The change of direction is sometimes 180° but frequently is a smaller angle, resulting in a random walk type motion. (B) Reorientation of P. citronellolis during reversal. The tracks are broader than those in (A) because the bacterium was above the plane of focus. (C) A slower strobing frequency allows comparison of the velocity in the forward and reverse directions. P. citronellolis apparently swims more slowly in the reverse direction. Cells were grown in minimal medium with glycerol as sole carbon source.*

[J. Bacteriol., **119**, 640 (1974)]

Pseudomonas citronellolis

Size $\sim$ **E. coli**

Light-switchable propulsion of active particles with reversible interactions

Propulsion direction reversable active particles by light modulation

Half-gold coated anatase TiO_2 particle

Active particle shows forward motion in the direction of TiO_2 side under the UV illumination, whereas the particle shows backward motion in the direction of gold-coated side under the green light illumination. The propulsion direction reversing is achieved by switching light illumination from UV to green, and vice-verse.

[Vutukuri, Lisicki, Lauga *et al. Nat Commun* **11**, 2628 (2020)]

Direction reversing active Brownian particle

In a small time interval Δt (in 2D)

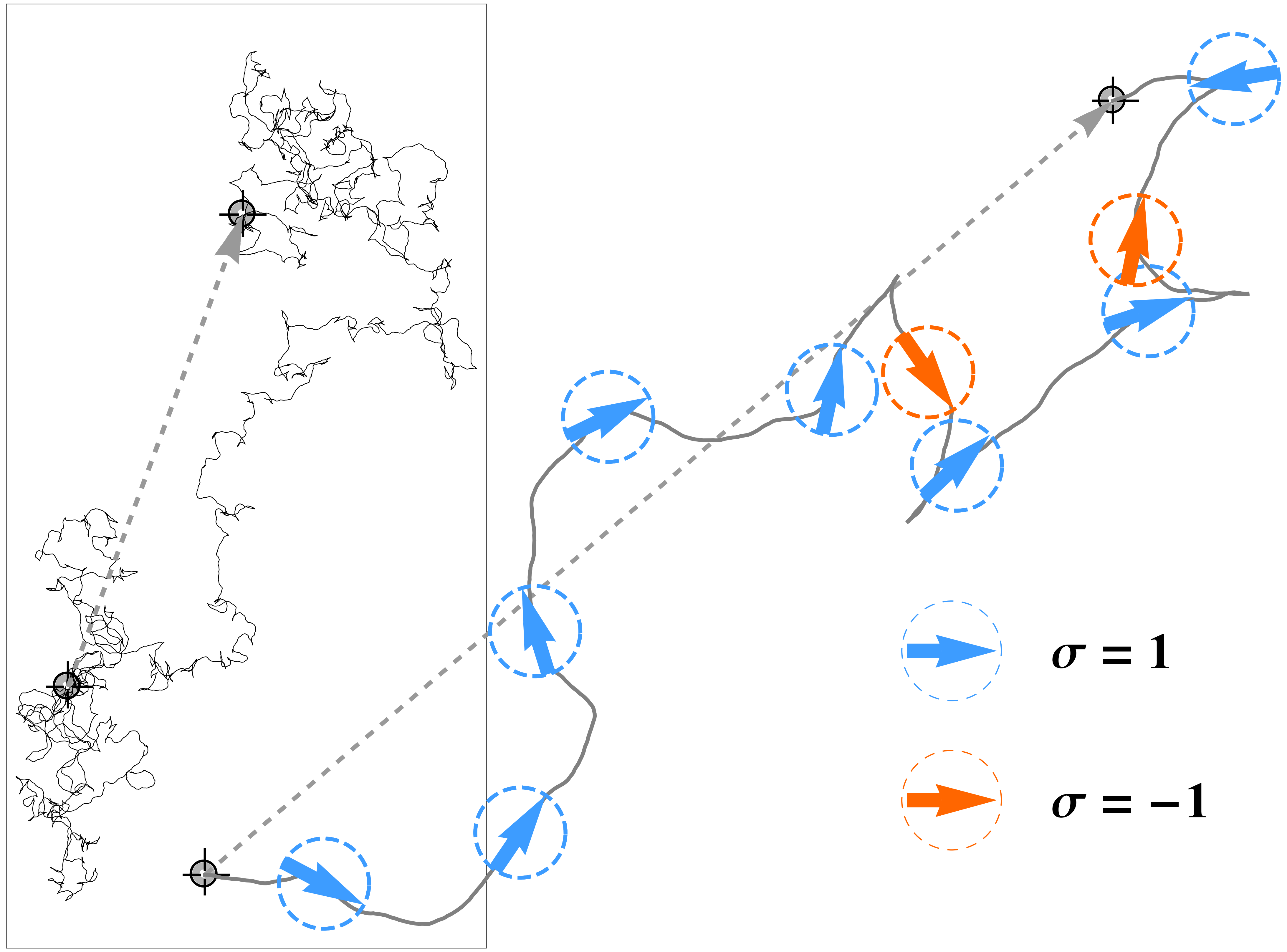
- **With probability $\gamma \Delta t$:** $\sigma \to -\sigma$ $\quad (\sigma = \pm 1)$

- **With probability $(1 - \gamma \Delta t)$**

$$\Delta x = \sigma\,[v_0 \cos\theta]\,\Delta t$$

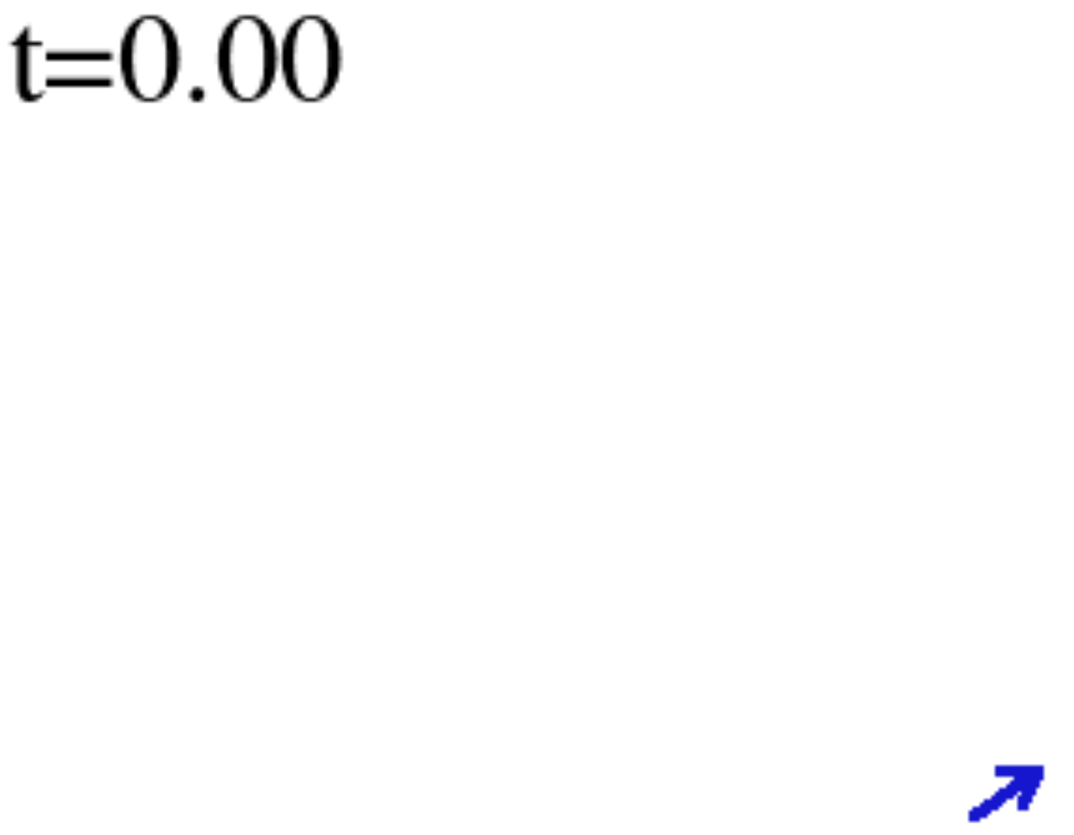
$$\Delta y = \sigma\,[v_0 \sin\theta]\,\Delta t$$

$$\Delta\theta = \sqrt{2D_{\mathrm{R}}\Delta t}\;\xi_\theta \qquad P(\xi_\theta) = \frac{e^{-\frac{1}{2}\xi_\theta^2}}{\sqrt{2\pi}}$$

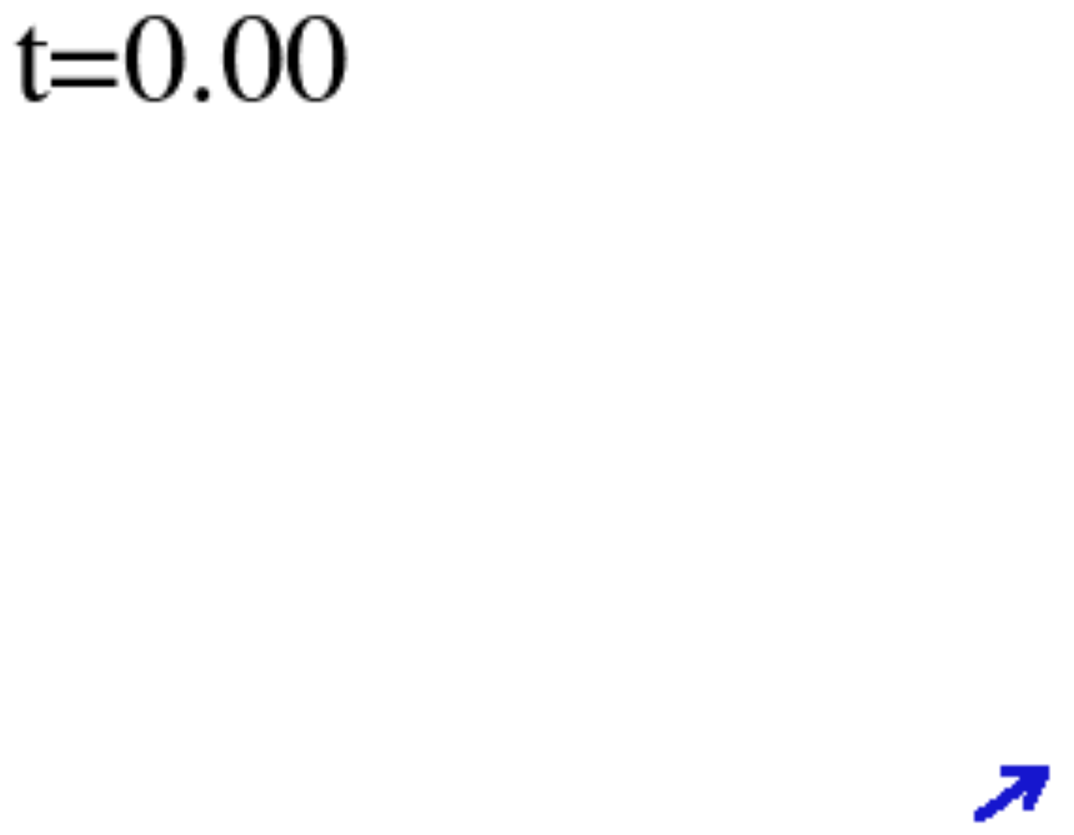


Dynamical evolution of the position distribution

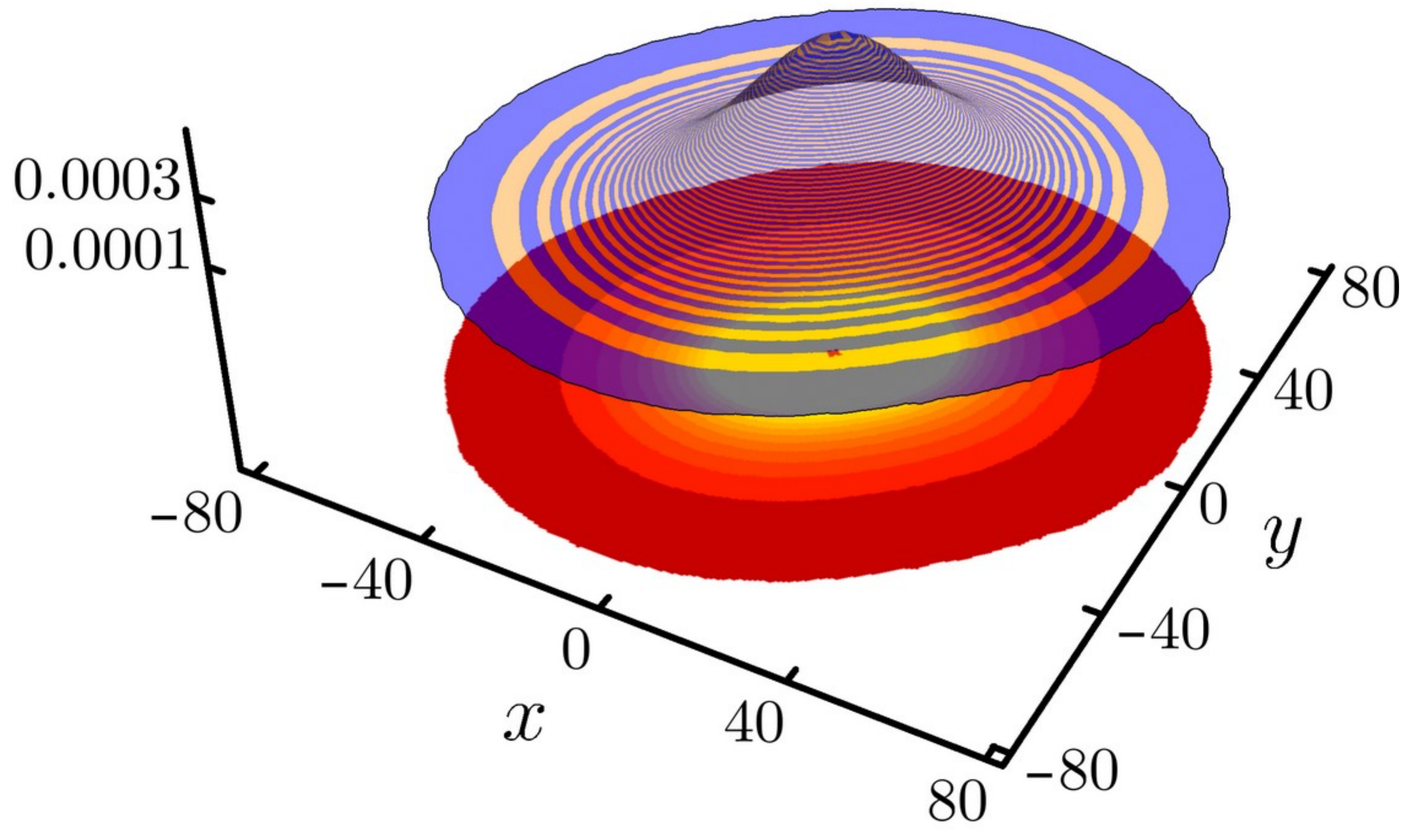
$\gamma > D_R$

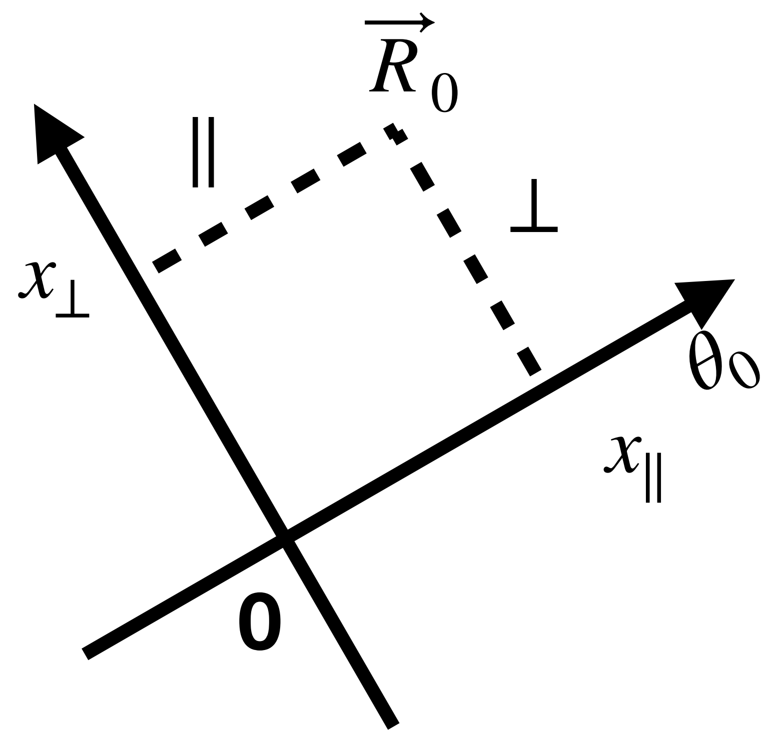


$\gamma < D_R$



Intermediate time: $\gamma^{-1} \ll t \ll D_R^{-1}$





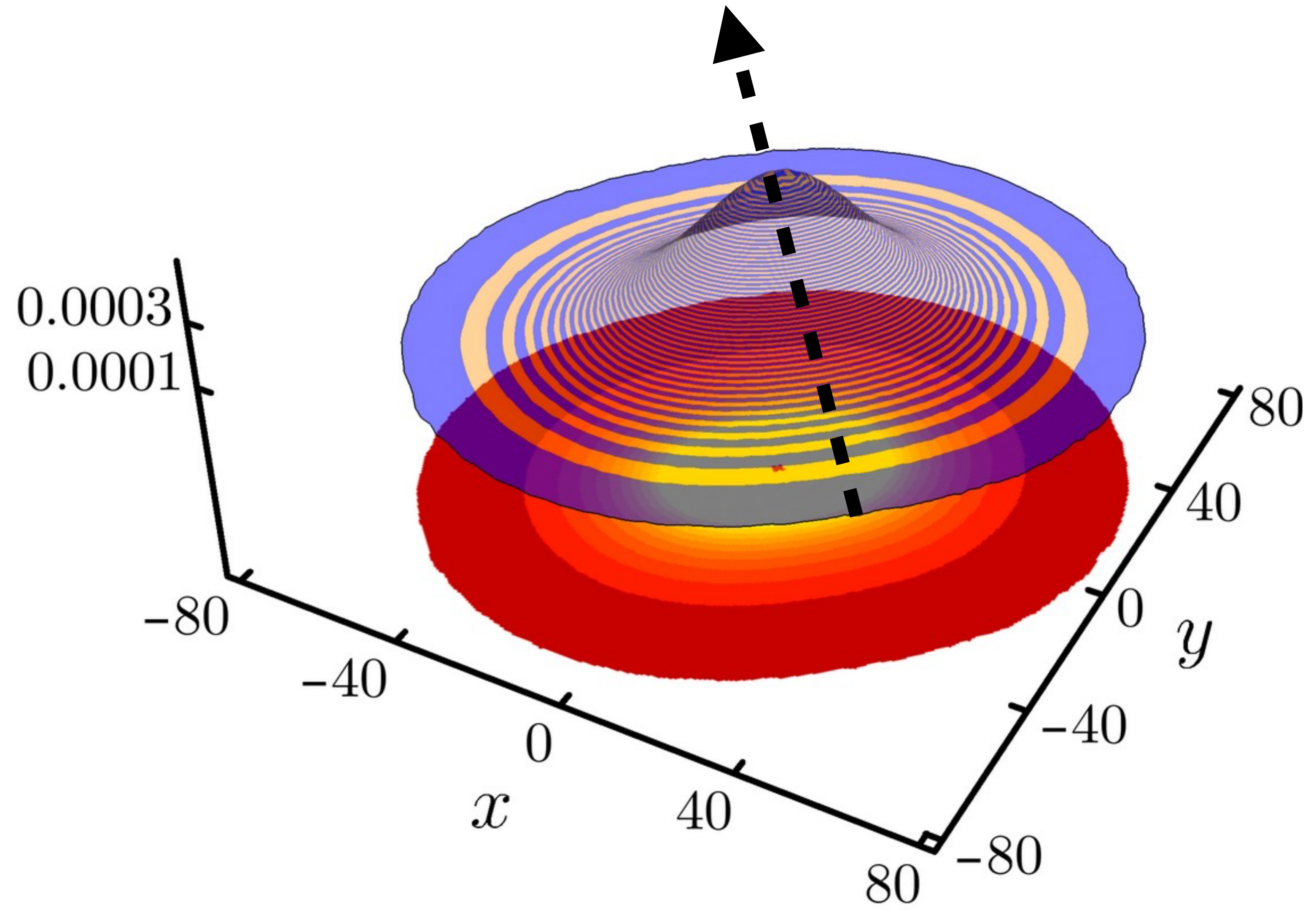
Brownian motion with a stochastic diffusion coefficient

$$\frac{dx_\perp}{dt} = \frac{v_0}{\sqrt{\gamma}} \phi \, \eta_\perp$$

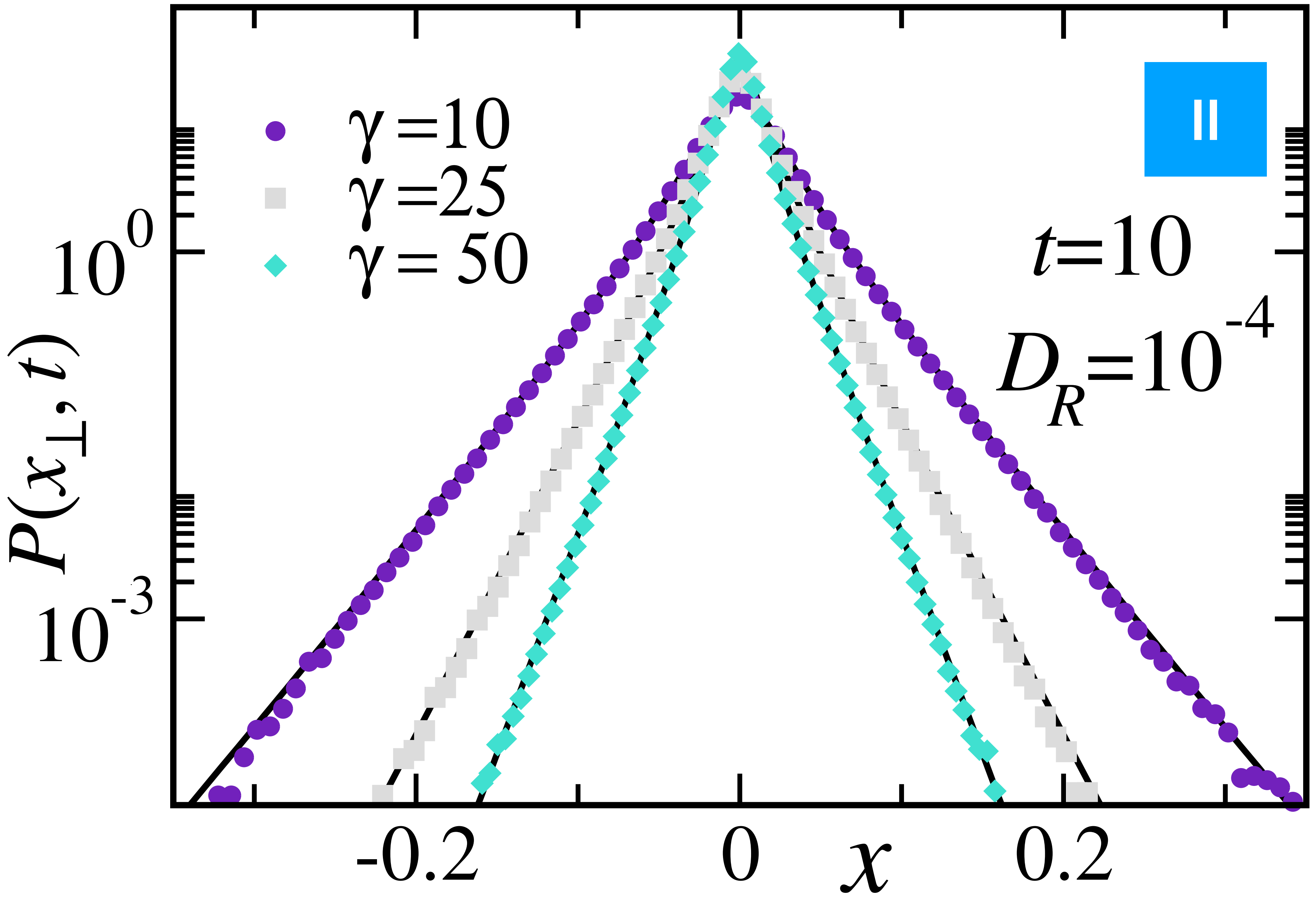
$$\frac{d\phi}{dt} = \sqrt{2D_R} \, \eta_\phi$$

$$\frac{\partial P}{\partial t} = \frac{v_0^2 \phi^2}{2\gamma} \frac{\partial^2 P}{\partial x_\perp^2} + D_R \frac{\partial^2 P}{\partial \phi^2}$$

Position distribution along the direction $\perp$ to θ_0



$$P(x_\perp, t) = \frac{1}{v_0 t}\sqrt{\frac{\gamma}{8D_R}}\, f\left(\frac{x_\perp}{v_0 t}\sqrt{\frac{\gamma}{8D_R}}\right)$$ **[ballistic scaling]**



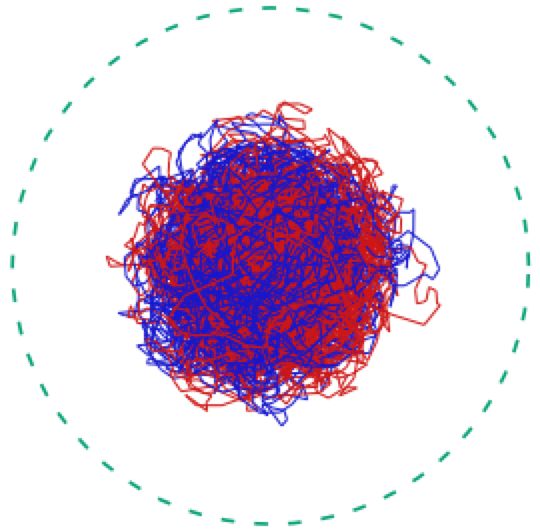
The scaling function is given by

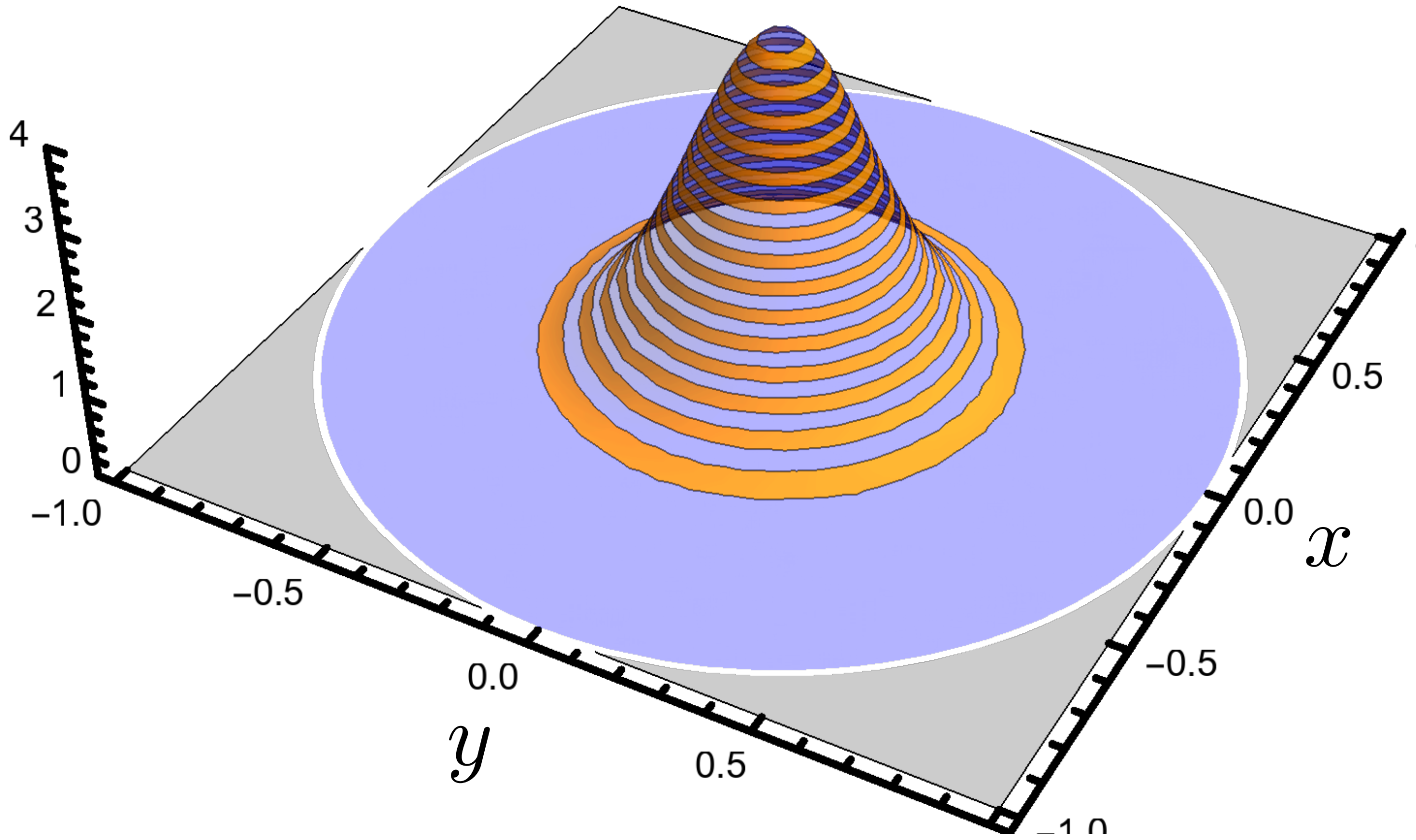
$$f(z) = \frac{1}{\sqrt{2\pi^3}}\,\Gamma\left(\frac{1}{4}+iz\right)\Gamma\left(\frac{1}{4}-iz\right) \sim \sqrt{\frac{2}{\pi|z|}}\, e^{-\pi|z|}$$

Soft Matt. (2021)

Stationary State in $U(\vec{r}) = \frac{\mu r^2}{2}$

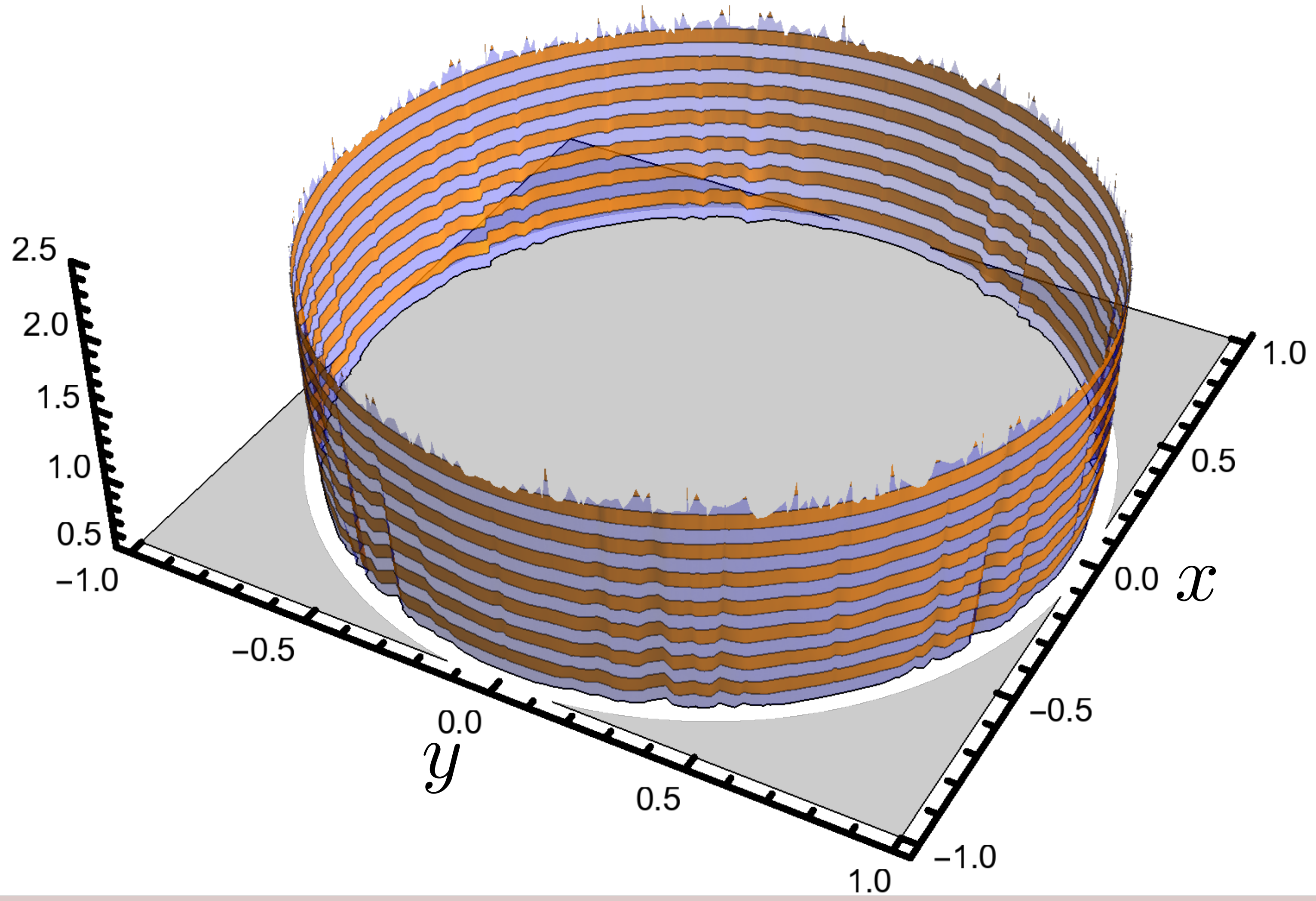
(a) Passive-I

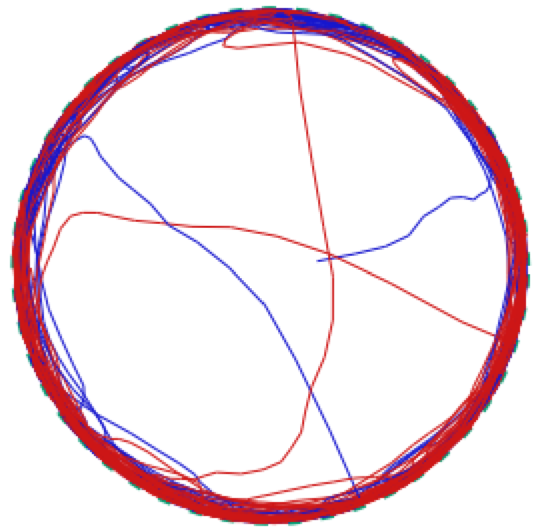




$D_R \gg \mu$,
for arbitrary γ

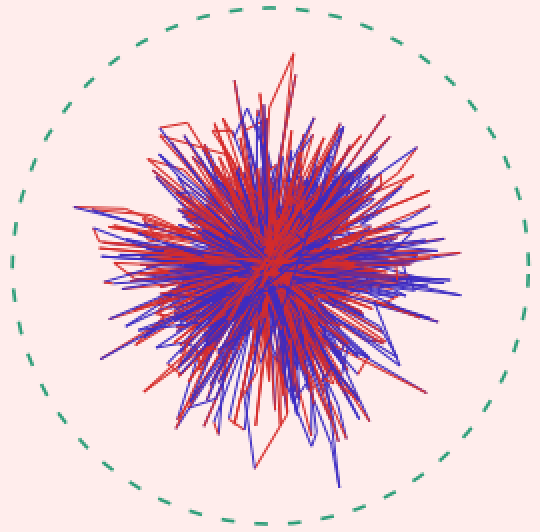
(b) Active-I

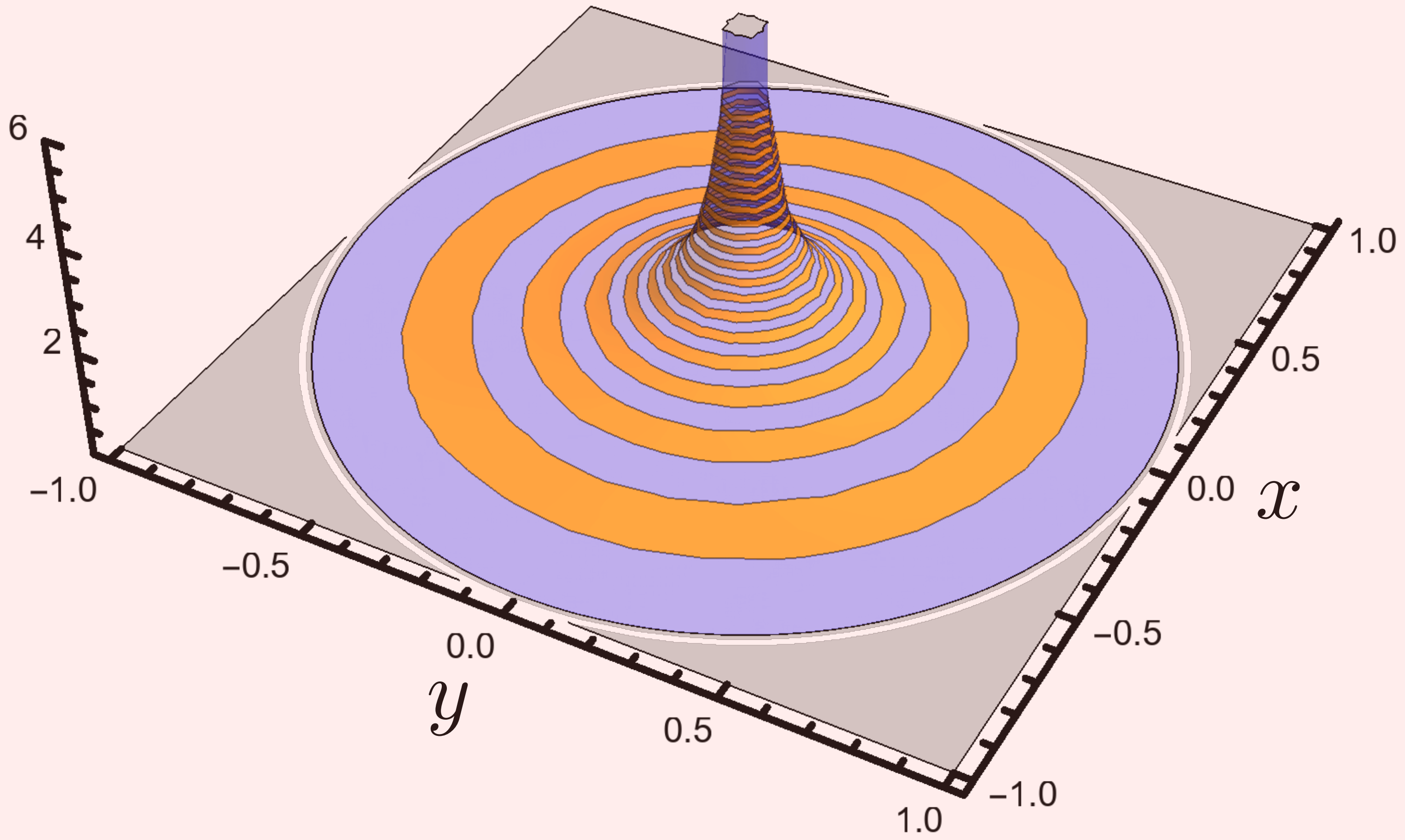




$\gamma \ll D_R \ll \mu$

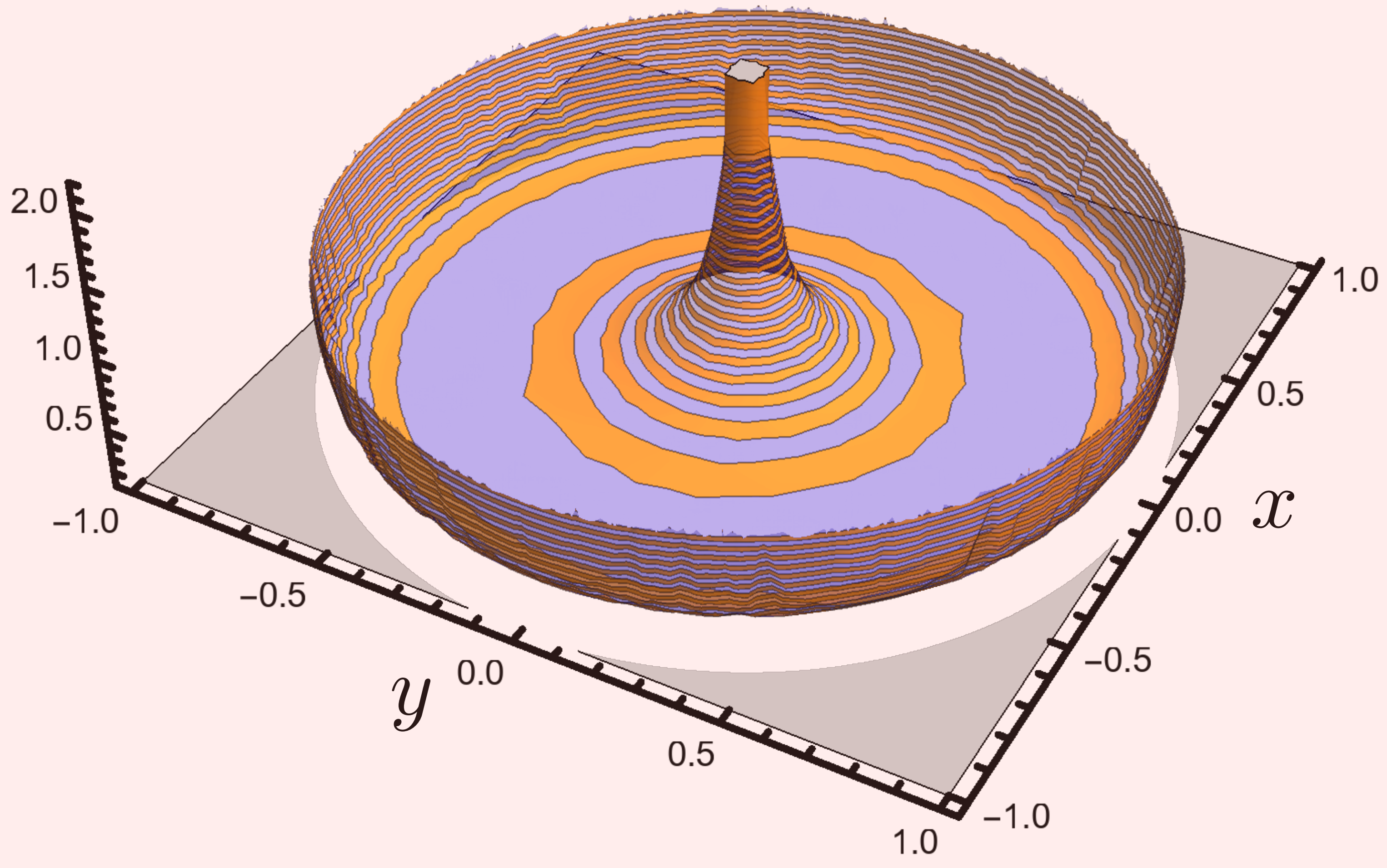
(c) Passive-II

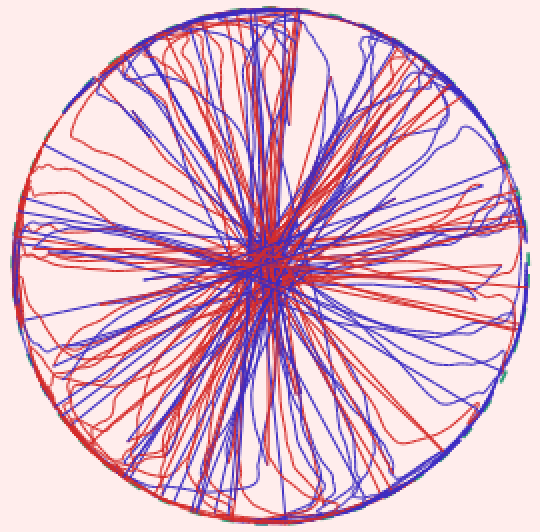




$\gamma > \mu \gg D_R$

(d) Active-II





$\mu > \gamma \gg D_R$

The steady state distribution in the active-II and passive-II phases

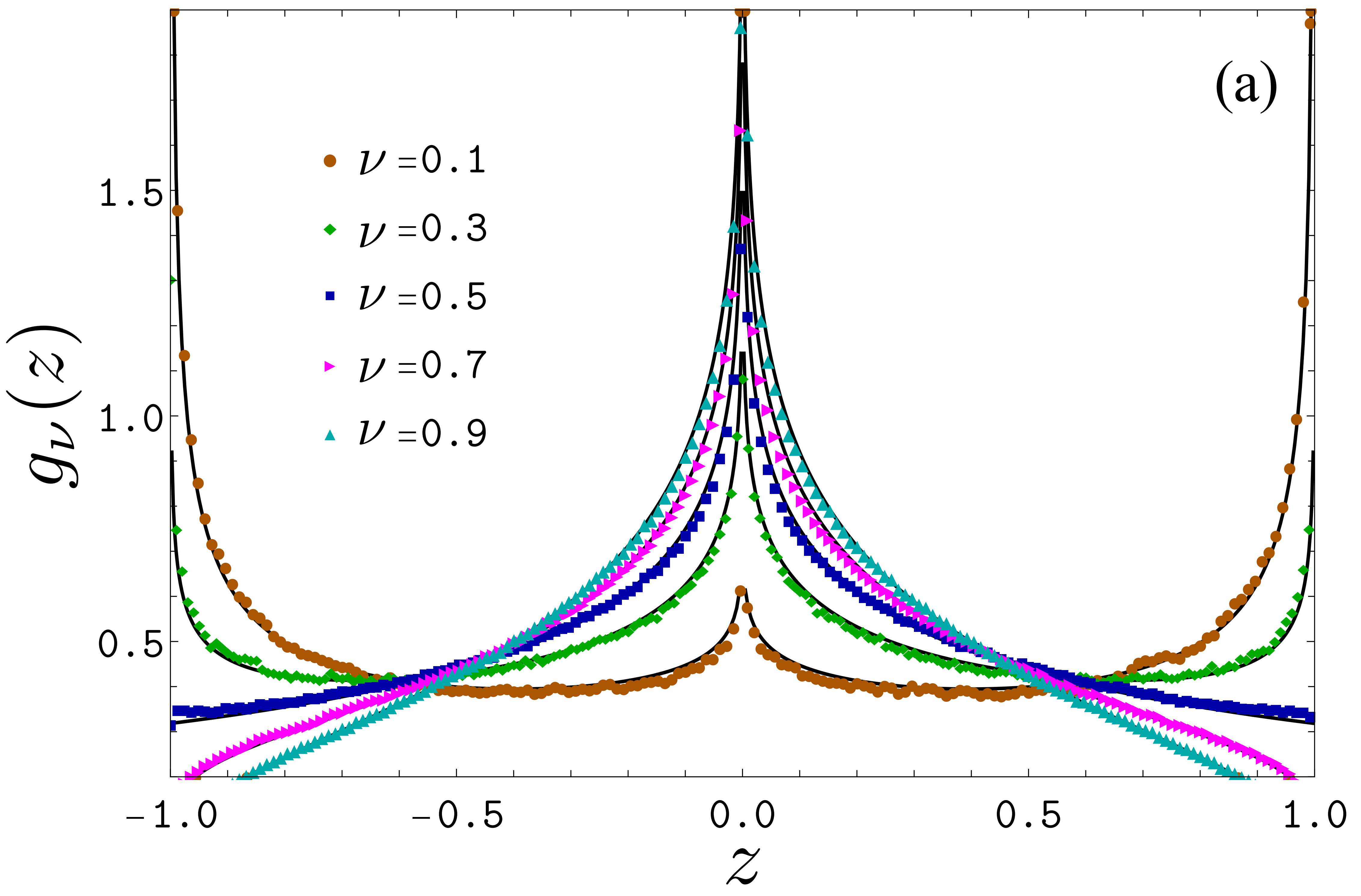
$$P(x,y) = \frac{1}{r_0^2} f_\nu\left(\frac{x}{r_0}, \frac{y}{r_0}\right) \quad \textbf{where} \quad f_\nu(z_1,z_2) = \frac{2^{1-2\nu}}{\pi B(\nu,\nu)} \frac{(1-z_1^2-z_2^2)^{\nu-1}}{\sqrt{z_1^2+z_2^2}} \Theta(1-z_1^2-z_2^2) \quad \textbf{and} \quad \nu = \gamma/\mu$$

Marginal: $P(x) \equiv \int P(x,y)\,dy = \frac{1}{r_0} g_\nu\left(\frac{x}{r_0}\right)$

where $g_\nu(z) = \frac{1}{\pi}(1-z^2)^{\nu-\frac{1}{2}} {}_2F_1\left(\frac{1}{2}, \nu, \nu+\frac{1}{2}, 1-z^2\right) \Theta(1-z^2)$

The behavior of the tails near $z = \pm 1$

$$g_\nu(z) \simeq \frac{1}{\pi} \times \begin{cases} \left[2(1-|z|)\right]^{-(1/2-\nu)} & 0 < \nu < 1/2, \\ 1 & \nu = 1/2, \\ \left[2(1-|z|)\right]^{\nu-1/2} & \nu > 1/2. \end{cases}$$



$D_R = 10^{-4}$ **and** $\mu = v_0 = 1 \implies r_0 = v_0/\mu = 1$

Universal central diverging peak in the active-II and passive-II phases

- Log-divergence at the center for all ν:

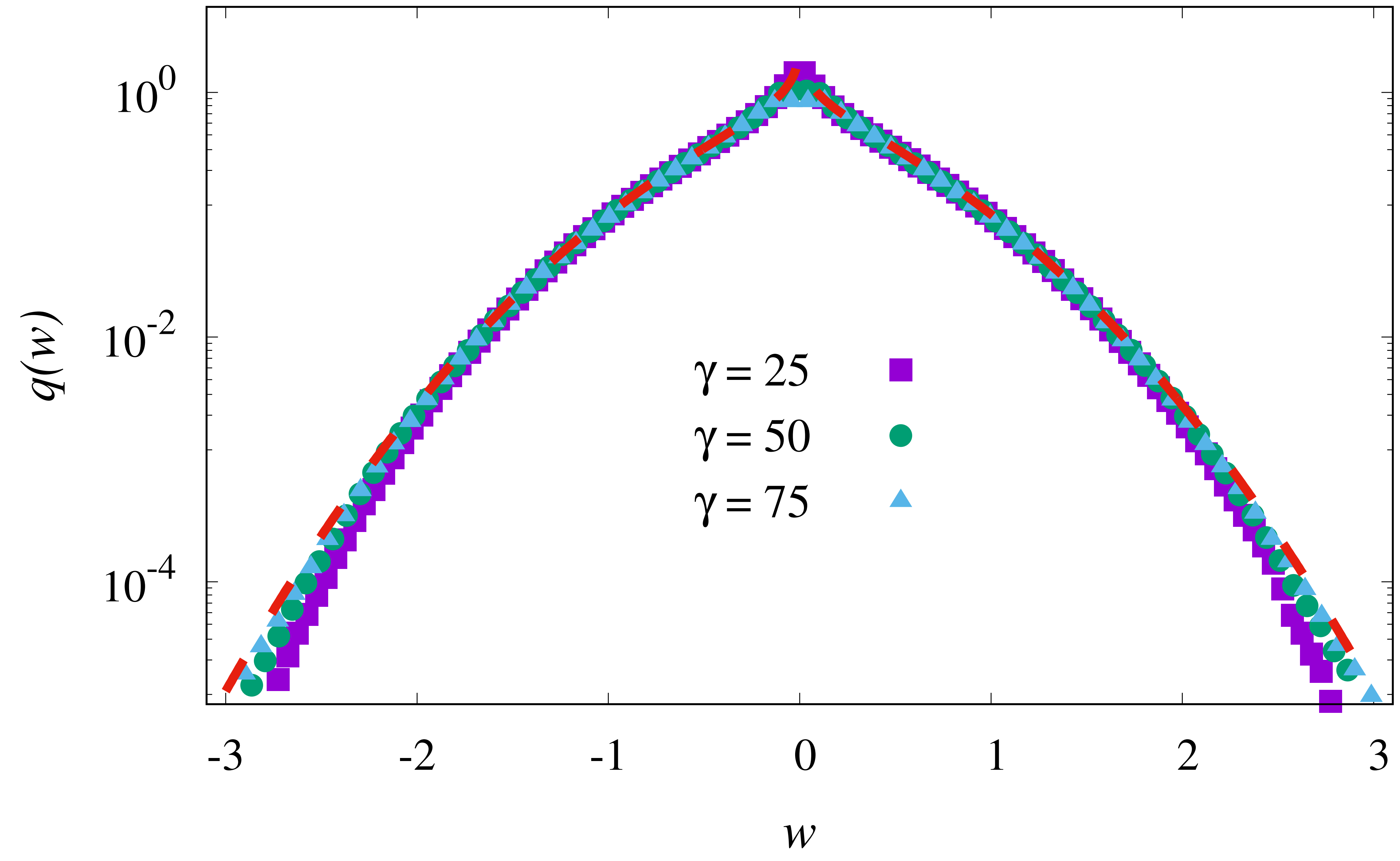
$$g_\nu(z) = -\frac{\Gamma\left(\nu+\frac{1}{2}\right)}{\pi^{3/2}\Gamma(\nu)}\left[\log\left(\frac{z^2}{4}\right)+E+\psi(\nu)\right]+O(z^2)$$

where $E = 0.5772\ldots$ and $\psi(\nu) = \Gamma'(\nu)/\Gamma(\nu)$

- **Boltzmann tail with a central divergence in the passive-II phase:** In the limit $\nu \to \infty, z \to 0$ keeping $z\sqrt{\nu}$ fixed, we get $g_\nu(z) = \sqrt{\nu}\, q\left(z\sqrt{\nu}\right)$,

$$q(w) = \frac{1}{\pi^{3/2}} K_0\left(\frac{w^2}{2}\right)\exp\left(-\frac{w^2}{2}\right)$$

Note: $w = x\sqrt{\mu}\Big/\sqrt{2D_{\mathrm{RT}}}$



$K_0(w^2/2) \sim \exp(-w^2/2)$ as $w \to \infty \implies q(w) \sim \exp(-w^2)$ **[Boltzmann]**

$K_0(w^2/2) = -\left[\log(w^2/4)+E\right]+O(w^4)$ as $w \to 0$.

Take-home message

Active particles having multiple time-scales can exhibit interesting novel features, due to the interplay between the times scales.