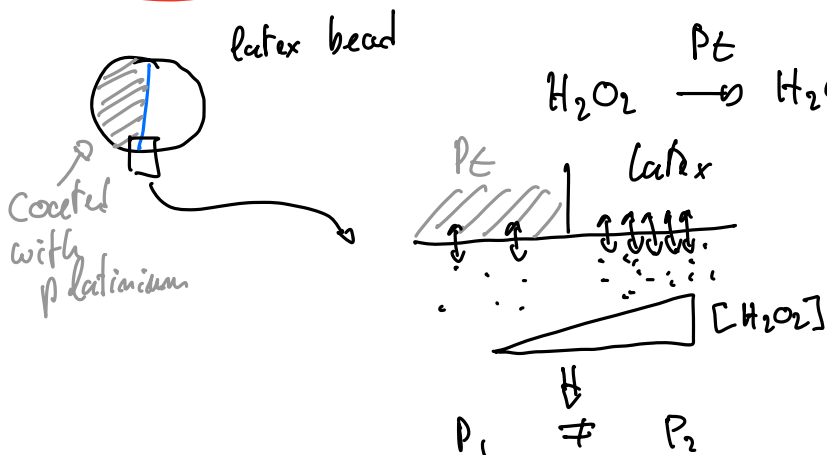


8.2) Active Brownian Particles

1

8.2.1) Model self-diffusiophoretic Janus colloids



Interactions between bead and solute $\leftrightarrow$ transfer of momentum

Gradient of interaction strengths $\leftrightarrow$ gradient of pressure in the fluid $\Rightarrow$ flow $\Rightarrow$ advect the particle $\Rightarrow$ self-propulsion

Everything you may want to know can be found in the R. Golestanian lecture notes
[Golestanian, arxiv:1909.03747]

In practice, many more ingredients (e.g. electrostatic interactions)
 $\rightarrow$ hard to predict speed or even direction of self-propulsion

Philosophically: Chemical reaction breaks time-reversal symmetry
Asymmetric coating breaks parity ($x \rightarrow -x$) $\Rightarrow$ ratchet.

Experimental reference

Latex / Pt: [Palacci et al, PRL 2010]

Am / Pt: [Theurkauff et al, PRL 2012]

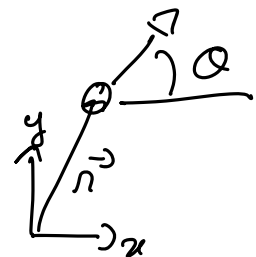
8.2.2) The model

$$\frac{d\vec{r}}{dt} = v_0 \vec{u}(\theta) + \sqrt{2D_t} \vec{\zeta} \quad (1)$$

$$\vec{u}(\theta) = (\cos\theta, \sin\theta)$$

$$\text{rotational diffusion } \dot{\theta} = \sqrt{2D_r} \xi \quad (2)$$

ζ_x, ζ_y and ξ are three Gaussian white noises.



2

$P(\vec{r}, \theta) = P(x, y, \theta)$ the probability to find the particle at x, y going in the direction θ at time t . (1) & (2) are Langevin dynamics $\Rightarrow$ dynamics of $P(\vec{r}, t)$ is a Fokker-Planck equation.

$$\begin{aligned} \partial_t P(x, y, \theta) &= -\frac{\partial}{\partial x} J_x - \frac{\partial}{\partial y} J_y - \frac{\partial}{\partial \theta} J_\theta \\ &= -\frac{\partial}{\partial x} \left[v_0 \cos \theta P - \frac{\partial}{\partial x} (D_\theta P) \right] - \frac{\partial}{\partial y} \left[v_0 \sin \theta P - \frac{\partial}{\partial y} (D_\theta P) \right] + \frac{\partial^2}{\partial \theta^2} (D_\theta P) \end{aligned}$$

$$\partial_t P(x, y, \theta) = -\vec{\nabla} \cdot \underbrace{\left[v_0 \vec{u}(\theta) P - \vec{\nabla} (D_\theta P) \right]}_{\substack{\text{Probability current} \\ \vec{r} \text{ space}}} - \frac{\partial}{\partial \theta} \underbrace{\left[-\frac{\partial}{\partial \theta} D_\theta P \right]}_{\substack{\text{probability current} \\ \text{in } \theta \text{ space}}}$$

Comment: If D_θ and D_n have as an origin the collision of the particle with an equilibrated fluid, they will be related. If D_n has an active origin, they need not be.

8.3 The relevant scales of active dynamics

8.3.1) The persistence time

Active particle starts with some orientation $\vec{u}_0$.

For how long does $\vec{u}(t)$ remains correlated to $\vec{u}_0$?

run and tumble particles in 2D:

$$\begin{aligned} \frac{d}{dt} \langle \vec{u}(0+t) \cdot \vec{u}(0) \rangle &= \frac{d}{dt} \langle \vec{u}(0+t) \rangle \cdot \vec{u}(0) \\ &= \frac{d}{dt} \int d^2 \vec{r} d\theta P(\vec{r}, \theta, t) \vec{u}(\theta) \cdot \vec{u}(0) \\ &= \int d^2 \vec{r} d\theta \frac{dP}{dt} \vec{u}(\theta) \cdot \vec{u}(0) \end{aligned}$$

(3)

$$\frac{dP}{dt} = - \underbrace{\nabla_{\vec{n}} \cdot [\vec{v}_p \vec{u}(\theta) P]}_{\int d^2 \vec{n} [\dots] = 0 \text{ since } P \xrightarrow{\vec{n} \rightarrow -\vec{n}} 0} - \alpha P + \frac{\alpha}{2\pi} g(\vec{n}) ; \quad g(\vec{n}) = \int d\theta P(\vec{n}, \theta)$$

$$\int d\theta g(\vec{n}) \vec{u}(\theta) = 0 \quad (\text{symmetry})$$

$$\Rightarrow \frac{d}{dt} \langle \vec{u}^2(\theta(t)) \cdot \vec{u}^2(\theta_0) \rangle = -\alpha \int d^2 n \int d\theta P(\vec{n}, \theta, t) \vec{u}^2(\theta) \cdot \vec{u}^2(\theta_0)$$

$$= -\alpha \langle \vec{u}^2(\theta(t)) \cdot \vec{u}^2(\theta_0) \rangle$$

$$\Rightarrow \langle \vec{u}^2(\theta(t)) \cdot \vec{u}^2(\theta_0) \rangle = \langle \vec{u}^2(\theta_0) \rangle e^{-\alpha t}$$

$$= e^{-\alpha t}$$

RTPs forget their orientation after a typical time $\tau = \frac{1}{\alpha}$

Active Brownian Particles

2D: $\dot{\theta} = \sqrt{2D_r} \xi$ Ito formula $\frac{d}{dt} \vec{u}(\theta(t)) = \frac{d\vec{u}}{d\theta} \dot{\theta} + D_r \frac{d^2 \vec{u}}{d\theta^2}$

$$\vec{u} = (\cos\theta, \sin\theta) \Rightarrow \frac{d\vec{u}}{d\theta} = (-\sin\theta, \cos\theta) \equiv \vec{u}^\perp(\theta) \Rightarrow \frac{d^2 \vec{u}}{d\theta^2} = -\vec{u}$$

$$\Rightarrow \frac{d}{dt} \vec{u} = \vec{u}^\perp \sqrt{2D_r} \xi - D_r \vec{u}$$

$$\frac{d}{dt} \langle \vec{u} \rangle \stackrel{\text{Ito}}{=} 0 - D_r \langle \vec{u} \rangle \text{ since } \langle \vec{u}^\perp(\theta(t)) \xi(t) \rangle \stackrel{\text{Ito}}{=} \langle \vec{u}^\perp(\theta(t)) \rangle$$

$$\times \underbrace{\langle \xi(t) \rangle}_{=0}$$

$$\text{Again } \langle \vec{u}^2(\theta(t)) \rangle = e^{-t/\tau} \langle \vec{u}^2(\theta_0) \rangle$$

$$\text{Here } \tau = \frac{1}{D_r} \quad ([\text{rotational diffusivity}] = \tau^{-1})$$

1 Dimension: Same path as RTP, & $\Delta_n \vec{u} = -(\alpha-1)\vec{u}$ leads to $\tau = \frac{1}{(\alpha-1)\Delta_n}$

(4)

6.3.2) Persistence length

$\vec{r} = \vec{v}_p(t)$ with $\vec{v}_p = v_p \vec{u}(0)$ & $v_p \in \mathbb{R}^+$ for ABP, RTP,

$$\vec{r}(t) - \vec{r}(0) = \int_0^t ds \vec{v}_p(s)$$

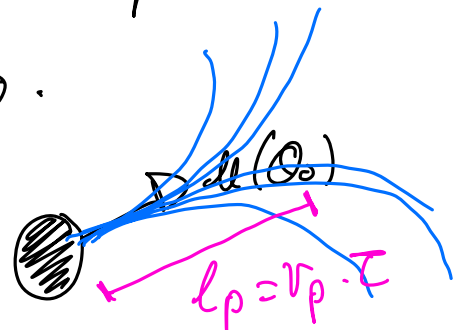
$$\begin{aligned} \langle \vec{r}(t) - \vec{r}(0) \rangle &= \int_0^t ds \langle \vec{v}_p(s) \rangle = \int_0^t ds e^{-s/\tau} \langle \vec{v}_p(0) \rangle \\ &= \langle \vec{v}_p(0) \rangle \cdot \left[-\tau e^{-s/\tau} \right]_0^t \\ &= \langle \vec{v}_p(0) \rangle \tau (1 - e^{-t/\tau}) \end{aligned}$$

For ABP & RTP, $\vec{v}_p = v_p \vec{u}(0)$

$$\langle (\vec{r}(t) - \vec{r}(0)) \cdot \vec{u}(0) \rangle = \ell_p (1 - e^{-t/\tau}) \xrightarrow{t \rightarrow \infty} \ell_p$$

where $\ell_p = v_p \cdot \tau \begin{cases} v_p \propto & \text{for RTP} \\ \propto v_p / (\alpha-1)\Delta_n & \text{for ABP} \end{cases}$

This measures the typical distance travelled by the particle along the direction it was facing at $t=0$.



8.3.3) Large scale diffusion

(5)

Formal solution of $x(t), y(t), \theta(t)$:

$$x(t) - x_0 = \int_0^t v_0 \cos[\theta(s)] ds + \int_0^t \sqrt{2D_\perp} z_x(s) ds$$

$$\theta(t) = \theta_0 + \int_0^t ds \sqrt{2D_\parallel} \zeta(s)$$

$$y(t) - y_0 = \int_0^t v_0 \sin[\theta(s)] ds + \int_0^t \sqrt{2D_\perp} z_y(s) ds$$

$$\theta(t) \text{ is a Wiener process} \Rightarrow \boxed{P(\theta(t) | \theta_0) = \frac{1}{\sqrt{4\pi D_\parallel t}} e^{-\frac{(\theta(t) - \theta_0)^2}{4D_\parallel t}}}$$

the mean-square displacement

$$P(\theta_0) = \frac{1}{2\pi};$$

$$\begin{aligned} \langle (x(t) - x_0)^2 \rangle &= \int_0^t du \int_0^t ds v_0^2 \langle \cos\theta(s) \cos\theta(u) \rangle + 2v_0 \sqrt{2D_\perp} \int_0^t du \int_0^t ds \langle \cos\theta(u) z_x(s) \rangle \\ &\quad + 2D_\perp \int_0^t du \int_0^t ds \underbrace{\langle z_x(u) z_x(s) \rangle}_{\delta(u-s)} \\ &\quad \underbrace{\quad}_{1} \\ &\quad \underbrace{\quad}_{2} \\ &\quad \underbrace{\quad}_{2D_\perp t} \end{aligned}$$

$= \langle \cos\theta(u) \rangle \underbrace{\langle z_x(s) \rangle}_{=0}$
 because $z_x(t)$ and $\theta(s)$ are statistically independent.

$$\begin{aligned} s > u \quad \partial_s \langle \cos\theta(s) \cos\theta(u) \rangle &= \langle \underbrace{-\sin\theta(s)}_{\sqrt{2D_\parallel} \zeta(s)} \cdot \cos\theta(u) \rangle - D_\parallel \langle \cos\theta(s) \cos\theta(u) \rangle \\ &\stackrel{\text{If } s > u}{=} \underbrace{\langle \sqrt{2D_\parallel} \zeta(s) \rangle}_0 \cdot \langle -\sin\theta(s) \rangle \end{aligned}$$

$$\Rightarrow \langle \cos\theta(s) \cos\theta(u) \rangle = \langle \cos^2\theta(u) \rangle e^{-D_\parallel(s-u)}$$

$$P(\theta_0) = \frac{1}{2\pi} \Rightarrow \text{isotropic } \langle \cos^2\theta(u) \rangle = \langle \sin^2\theta(u) \rangle$$

$$\text{and } \langle \cos^2(u) + \sin^2(u) \rangle = 1 \Rightarrow \langle \cos^2\theta(u) \rangle = \frac{1}{2}$$

$$s > u \quad \langle \cos\theta(s) \cos\theta(u) \rangle = \frac{1}{2} e^{-D_\parallel(s-u)}$$

$$u > s \quad \langle \cos\theta(s) \cos\theta(u) \rangle = \frac{1}{2} e^{-D_\parallel(u-s)}$$

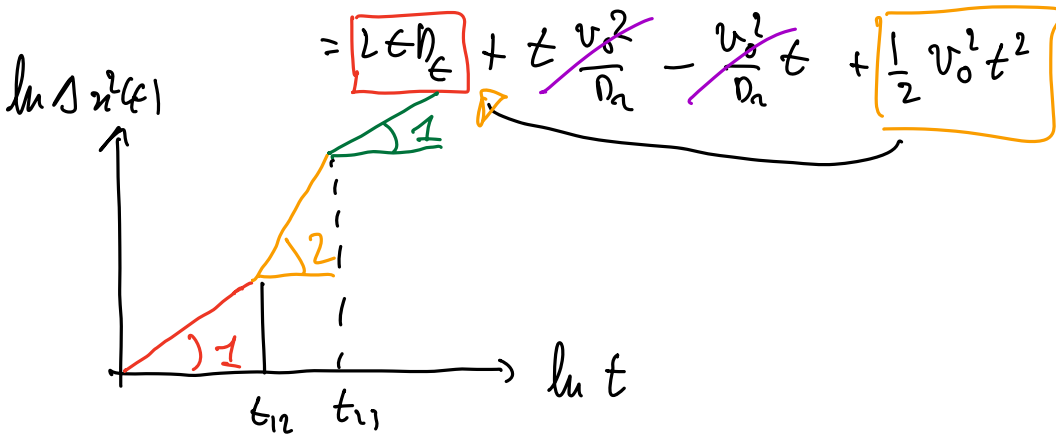
(6)

$$\begin{aligned}
\langle (x(t) - x(0))^2 \rangle &= 2D_E t + \frac{v_0^2}{2} \int_0^t du \left[\underbrace{\int_0^u ds e^{-D_n(u-s)}}_{e^{-D_n u} \left(\frac{e^{D_n u} - 1}{D_n} \right)} + \underbrace{\int_u^t ds e^{-D_n(s-u)}}_{e^{D_n u} \frac{e^{-D_n t} - e^{-D_n u}}{-D_n}} \right] \\
&= 2D_E t + \frac{v_0^2}{2D_n} \int_0^t du \left[1 - e^{-D_n u} - e^{D_n(u-t)} + 1 \right] \\
&= 2t \left[D_E + \frac{v_0^2}{2D_n} \right] + \frac{v_0^2}{2D_n} \left\{ \frac{e^{-D_n t} - 1}{D_n} - \frac{1 - e^{-D_n t}}{D_n} \right\}
\end{aligned}$$

$$\langle \Delta x^2(t) \rangle = 2t \left[D_E + \frac{v_0^2}{2D_n} \right] + \frac{v_0^2}{D_n^2} \{ e^{-D_n t} - 1 \}$$

$$t \rightarrow \infty \quad \Delta x^2(t) \sim \boxed{2D_{\text{eff}} t}; \quad D_{\text{eff}} = D_E + \frac{v_0^2}{2D_n}$$

$$t \rightarrow 0 \quad \Delta x^2(t) = 2tD_E + t \frac{v_0^2}{D_n} + \frac{v_0^2}{D_n^2} \left\{ \cancel{1 - D_n t} + \frac{1}{2} D_n^2 t^2 - \cancel{1} \right\}$$



Three successive regimes

① translational diffusion $\Delta x^2 \sim t D_n$

② ballistic motion $\Delta x^2 \sim t^2 v_0^2$

③ rotational diffusion makes diffusion win again $\Delta x^2 \sim D_{\text{eff}} t$

Comment: the average in $\langle \Delta x^2(t) \rangle$ represent averages over

$\rightarrow O_0$

$\rightarrow$ the realisations of $\{t\}, m_x(t), m_y(t)$.

(i) t_{12} such that $2 t_{12} D_e = \frac{1}{2} v_0^2 t_{12}^2 \Rightarrow t_{12} = \frac{4 D_e}{v_0^2} \rightarrow$ tells you the time scale at which ballistic motion at speed v_0 beats diffusion at diffusivity D_e .

(ii) t_{23} such that $\frac{1}{2} v_0^2 t_{23}^2 = 2 D_{eff} t_{23} = \frac{v_0^2}{D_a} t_{23}$ when $D_{eff} \gg D_e$
 $t_{23} = \frac{2}{D_a} = 2\tau_i$

(iii) $t_{23} > t_{12} \Leftrightarrow \tau > \frac{2 D_e}{v_0^2} \Leftrightarrow v_0^2 \tau^2 > 2 D_e \tau \Leftrightarrow \ell_p > \sqrt{2 D_e \tau}$
 $\Leftrightarrow$ self prop further over τ than diffusion over τ .

(iv) When $t \gg \tau$, the persistence time, the active dynamics has been randomized by the rotational diffusion and it amounts to a random walk of diffusivity D_{eff} .

§.4) External potentials

§.4.1) Stochastic thermodynamics

Underdamped active dynamics

$$\dot{\vec{r}} = \vec{v} ; m \dot{\vec{v}} = -\gamma \vec{v} - \vec{\nabla} V_{ext}(\vec{r}) + \sqrt{2\gamma kT} \vec{\zeta} + \underbrace{\vec{f}_p}_{\substack{\text{propulsive force}}}$$

$E = \frac{1}{2} v^2 + V(\vec{r})$. Along a trajectory $\frac{dE}{dt} = -\gamma v^2 + \frac{d}{dt} \frac{\gamma kT}{m} + \sqrt{2\gamma kT} \vec{\zeta} \cdot \vec{v} + \vec{f}_p \cdot \vec{v}$

$$\frac{d}{dt} \langle E \rangle = \underbrace{-\gamma \langle v^2 \rangle}_{\text{dissipation}} + \underbrace{\frac{d}{dt} \frac{\gamma kT}{m} + \langle \vec{f}_p \cdot \vec{v} \rangle}_{\substack{\omega_p \\ \text{injection of energy}}}$$

In general, it is natural to expect that $\vec{v}$ closely follows $\vec{f}_p$ so that $\vec{f}_p \cdot \vec{v} > 0$. ω_p measures the power injected in the system by the active force.

This disconnection between injection and dissipation of energy drives active particles out of equilibrium.

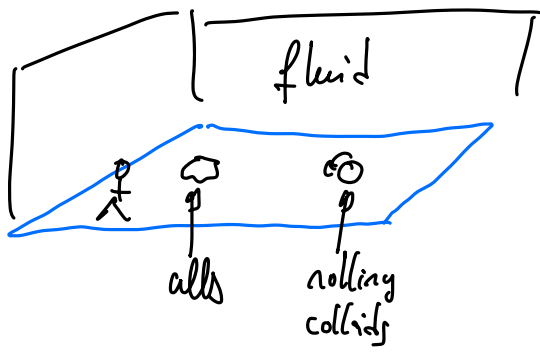
Comments:

* $\vec{f}_p(t)$ enters $\frac{d\mathcal{E}}{dt}$ through the dissipated power $\omega_p = \vec{f}_p \cdot \vec{v}$
 $\Rightarrow \vec{f}_p$ is a non-conservative force

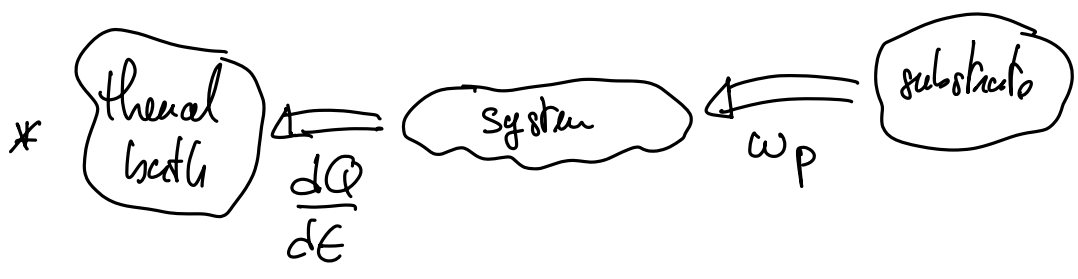
* $\langle \frac{d\mathcal{E}}{dt} \rangle = 0$ in steady-state

$$\langle \sigma v^2 \rangle - \frac{d\sigma_{\text{tot}}}{dt} = \frac{dQ}{dt} = \langle \vec{f}_p \cdot \vec{v} \rangle \equiv \omega_p$$

On average, the power injected by the active force ω_p is balanced by the energy dissipated in the thermal bath.



the particles are self-propelled by exchanging momentum with a substrate, and also interact with a surrounding fluid.



In this sense, the dissipation w_p characterizes the departure from thermal equilibrium of the system and it thus attracted a lot of interest.

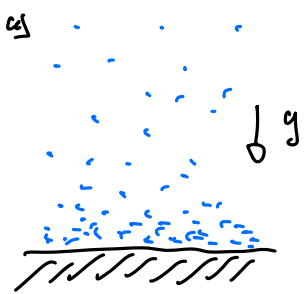
9

Conclusion: Since we have disconnected injection & dissipation of energy, the dynamics need not relax towards $P(\vec{r}) = e^{-\beta V(\vec{r})} / Z$

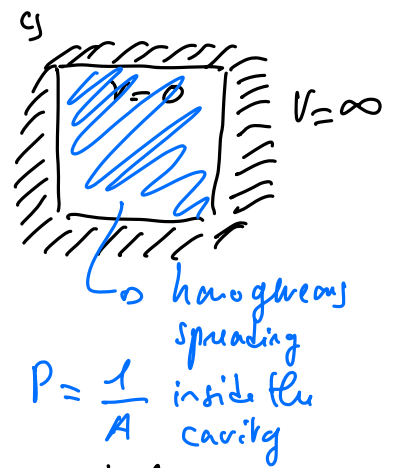
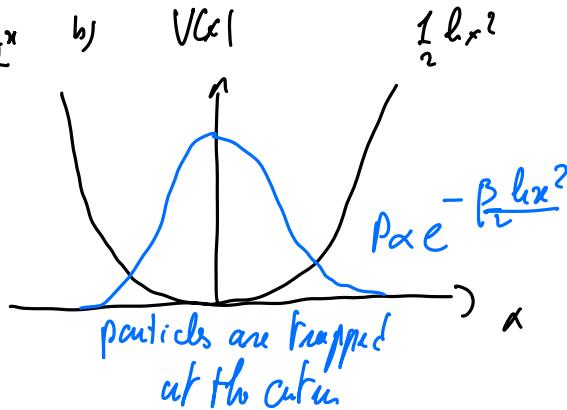
6.42) Steady state of non interacting particles in the presence of an external potential

Q: What the physics that one should expect in the presence of external potentials.

Equilibrium:



$$P(x) \propto e^{-\frac{\Delta m g x}{kT}}$$



This question is not only important conceptually to distinguish active particles from passive ones but also experimentally because external potentials are the way we interact with active particles and control them.

as Sedimentation

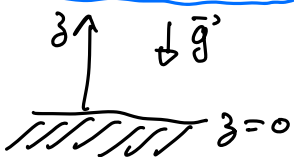
A bunch of exact results and some experiments on the sedimentation of active particles.

$$\vec{v} = -v_s \hat{z} + \vec{v}_p \quad (\hat{z} \text{ unit vector along } z\text{-axis})$$

$$\vec{v}_s \text{ Stokes sedimentation speed} \quad v_s = \mu \Delta m g = -\partial_z V_{\text{gravity}}(z) \times \mu$$

$$\vec{v}_p \text{ self-propulsion speed} \quad \text{speed at which particle falls at } T=0$$

Run and tumble particles: $P_s(z) = \frac{1}{Z} e^{-\gamma z} \Rightarrow$ always an exponential profile away from the confining boundary.



$$\lambda_{1D} = \frac{v_s \alpha}{v_p^2 - v_s^2} \quad \text{where } v_p = |\vec{v}_p| \text{ and } \alpha \text{ is the tumbling rate}$$

(10)

$$\lambda_{2D} = \frac{2\alpha v_s}{v_p^2 - v_s^2}$$

$$\lambda_{3D} \rightarrow \text{no explicit formula, solution of } \frac{\lambda(v_p + v_s) + \alpha}{\lambda(v_p - v_s) + \alpha} = e^{2\frac{\lambda v_p}{\alpha}}$$

Refs: Tailleur, Cates, PRL 2008
Cates, Tailleur, EPL 2009
Sole, Cates, Tailleur, EPJST 2015

& references therein.

Comments:

* $v_s \rightarrow v_p$; $\lambda \rightarrow \infty$; the average sedimentation length
 $\ell \rightarrow 0 \Rightarrow$ gravitational collapse



$\rightarrow$ Make sense because when $v_s > v_p$, $\dot{\vec{r}} \cdot \hat{\vec{z}} < 0 \Rightarrow$ whatever the direction in which the particle is looking, it is going down.

$\rightarrow$ add translational noise $\dot{\vec{r}} = \vec{v}_p + \vec{v}_s + \sqrt{2\alpha\tau} \vec{e}$
 $\hookrightarrow$ regularize a finite sedimentation length.

$$* v_s \ll v_p \Rightarrow \lambda \simeq \frac{\alpha v_s}{v^2} \Rightarrow P \propto e^{-\frac{\mu \Delta g z \alpha}{v^2}} \equiv e^{-\frac{\Delta g z}{kT_{\text{eff}}}}$$

$$kT_{\text{eff}} \equiv \frac{v^2}{\alpha \mu} \Rightarrow \text{effective temperature regime}$$