6.3.2) Persistence length

$\dot{\vec{r}} = \vec{v}_p(t)$ with $\vec{v}_p = v_p \, \vec{u}(\theta)$ & $v_p \in \mathbb{R}^+$ for ABPs, RTPs

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

$$\langle \vec{r}(t) - \vec{r}(0) \rangle = \int_0^t ds \, \langle \vec{v}_p(s) \rangle = \int_0^t ds \, e^{-t/\tau} \langle \vec{v}_p(0) \rangle$$

$$= \langle \vec{v}_p(0) \rangle \cdot \left[-\tau e^{-s/\tau} \right]_0^t$$

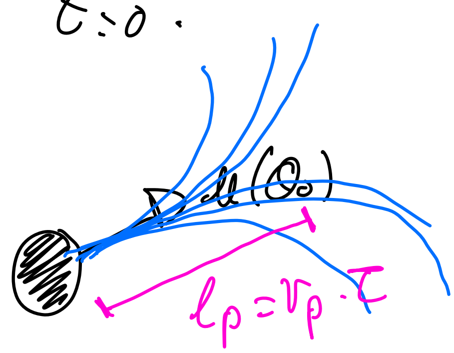
$$= \langle \vec{v}_p(0) \rangle \tau \left(1 - e^{-t/\tau}\right)$$

For ABPs & RTPs, $\vec{v}_p = v_p \, \vec{u}(\theta_0)$

$$\langle (\vec{r}(t) - \vec{r}(0)) \cdot \vec{u}(\theta_0) \rangle = \ell_p \left(1 - e^{-t/\tau}\right) \xrightarrow[t \to +\infty]{} \ell_p$$

where $\ell_p = v_p \cdot \tau \begin{cases} \to v_p/\alpha & \text{for RTPs} \\ \to v_p/_{(d-1)D_r} & \text{for ABPs} \end{cases}$

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



8.3.3) Large scale diffusion

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

$$x(t)-x_0=\int_0^t v_0\cos[\theta(s)]\,ds+\int_0^t\sqrt{2D_t}\,\eta_x(s)\,ds \qquad \theta(t)=\theta_0+\int_0^t ds\,\sqrt{2D_r}\,\xi(s)$$

$$y(t)-y_0=\int_0^t v_0\sin[\theta(s)]\,ds+\int_0^t\sqrt{2D_t}\,\eta_y(s)\,ds$$

$\theta(t)$ is a Wiener process $\Rightarrow$ $\boxed{P(\theta(t)\,|\,\theta_0)=\dfrac{1}{\sqrt{4\pi D_r t}}\,e^{-\frac{(\theta(t)-\theta_0)^2}{4Dt}}}$

The mean-square-displacement

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

$$\langle(x(t)-x_0)^2\rangle=\int_0^t du\int_0^t ds\, v_0^2\langle\cos\theta(s)\cos\theta(u)\rangle+2v_0\sqrt{2D_t}\int_0^t du\int_0^t ds\,\underbrace{\langle\cos\theta(u)\,\eta_x(s)\rangle}_{=\langle\cos\theta(u)\rangle\underbrace{\langle\eta_x(s)\rangle}_{=0}}$$

$$+\underbrace{2D_t\underbrace{\int_0^t du\underbrace{\int_0^t ds\,\underbrace{\langle\eta_x(u)\,\eta_x(s)\rangle}_{\delta(u-s)}}_{1}}_{t}}_{2D_t t}$$

because $\eta_x(t)$ and $\theta(s)$ are statistically independent.

$s>u$ $\quad \partial_s\langle\cos\theta(s)\cos\theta(u)\rangle=\langle-\sin\theta(s).\underbrace{\dot\theta(s)}_{\sqrt{2D_r}\,\xi(s)}.\cos\theta(u)\rangle-D_r\langle\cos\theta(s)\cos\theta(u)\rangle$

$$\overset{\text{Ito}}{\underset{s>u}{=}}\underbrace{\langle\sqrt{2D_r}\,\xi(s)\rangle}_{0}.\langle-\sin\theta(s)\rangle$$

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

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

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

$s>u$ $\quad\langle\cos\theta(s)\cos\theta(u)\rangle=\dfrac{1}{2}\,e^{-D_r(s-u)}$

$u>s$ $\quad\langle\cos\theta(s)\cos\theta(u)\rangle=\dfrac{1}{2}\,e^{-D_r(u-s)}$

3

$$\langle (x(t)-x(0))^2\rangle = 2D_t \cdot t + \frac{v_0^2}{2}\int_0^t du\left[\underbrace{\int_0^u ds\, e^{-D_r(u-s)}}_{e^{-D_r u}\left(\frac{e^{D_r u}-1}{D_r}\right)} + \underbrace{\int_u^t ds\, e^{-D_r(s-u)}}_{+e^{D_r u}\frac{e^{-D_r t}-e^{-D_r u}}{-D_r}}\right]$$

$$= 2D_t t + \frac{v_0^2}{2D_r}\int_0^t du\left[1 - e^{-D_r u} - e^{D_r(u-t)} + 1\right]$$

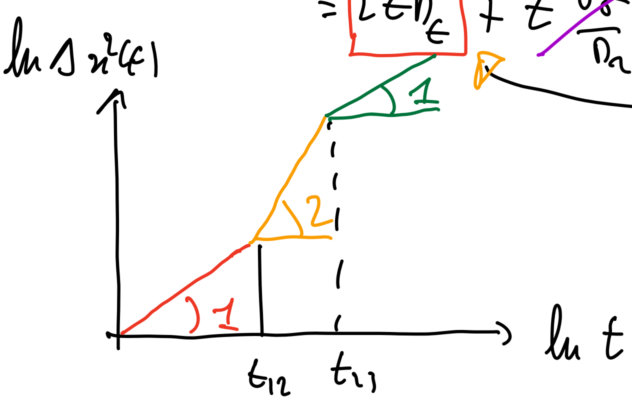
$$= 2t\left[D_t + \frac{v_0^2}{2D_r}\right] + \frac{v_0^2}{2D_r}\left\{\frac{e^{-D_r t}-1}{D_r} - \frac{1-e^{-D_r t}}{D_r}\right\}$$

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

$t \to \infty$ $\quad \Delta x^2(t) \sim \boxed{2D_{eff}t}$; $\quad D_{eff} = D_t + \frac{v_0^2}{2D_r}$

$t \to 0$ $\quad \Delta x^2(t) = 2tD_t + t\frac{v_0^2}{D_r} + \frac{v_0^2}{D_r^2}\left\{\cancel{1} - D_r t + \frac{1}{2}D_r^2 t^2 \cancel{-1}\right\}$

$$= \boxed{2tD_t} + \cancel{t\frac{v_0^2}{D_r}} - \cancel{\frac{v_0^2}{D_r}t} + \boxed{\frac{1}{2}v_0^2 t^2}$$



three successive regimes

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

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

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

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

$\to \theta_0$

$\to$ the realisations of $\xi(t), \eta_x(t), \eta_y(t)$.

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

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

$$t_{23} = \frac{2}{D_r} = 2\tau;$$

(iii) $t_{23} > t_{12} \Leftrightarrow \quad \tau > \frac{2D_t}{v_0^2} \Leftrightarrow v_0^2 \tau^2 > 2 D_t \tau \Leftrightarrow l_p > \sqrt{2 D_t \tau}$

$\Leftrightarrow$ self propel farther 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}.

8.4) External potentials

8.4.1) Stochastic thermodynamics

Underdamped active dynamics

$$\dot{\vec{r}} = \vec{v} \; ; \; m\dot{\vec{v}} = -\gamma \vec{v} - \vec{\nabla} V_{ext}(\vec{r}) + \sqrt{2\gamma k_B T}\, \vec{\eta} + \underbrace{\vec{f}_p}_{\text{propulsion force}}$$

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

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

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:

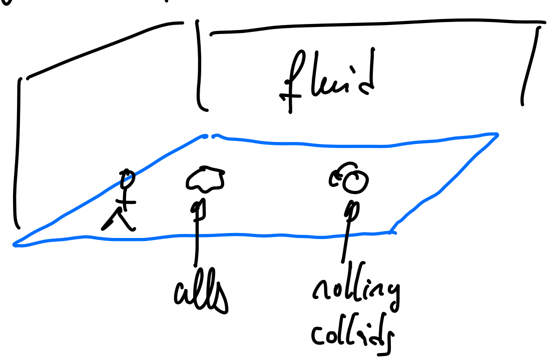
* $\vec{f}_p(t)$ enters $\frac{dE}{dt}$ through the dissipated power $w_p = \vec{f}_p \cdot \vec{v}$

  $\Rightarrow \vec{f}_p$ is a non-conservative force

* $\left\langle \frac{dE}{dt} \right\rangle = 0$ in steady-state

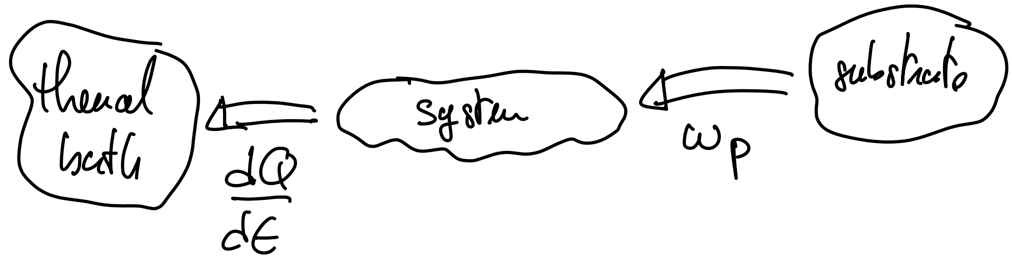
$$\langle \gamma v^2 \rangle - d\frac{\gamma k_B T}{m} = \frac{dQ}{dt} = \langle \vec{f}_p \cdot \vec{v} \rangle \equiv \omega_p$$

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.

*



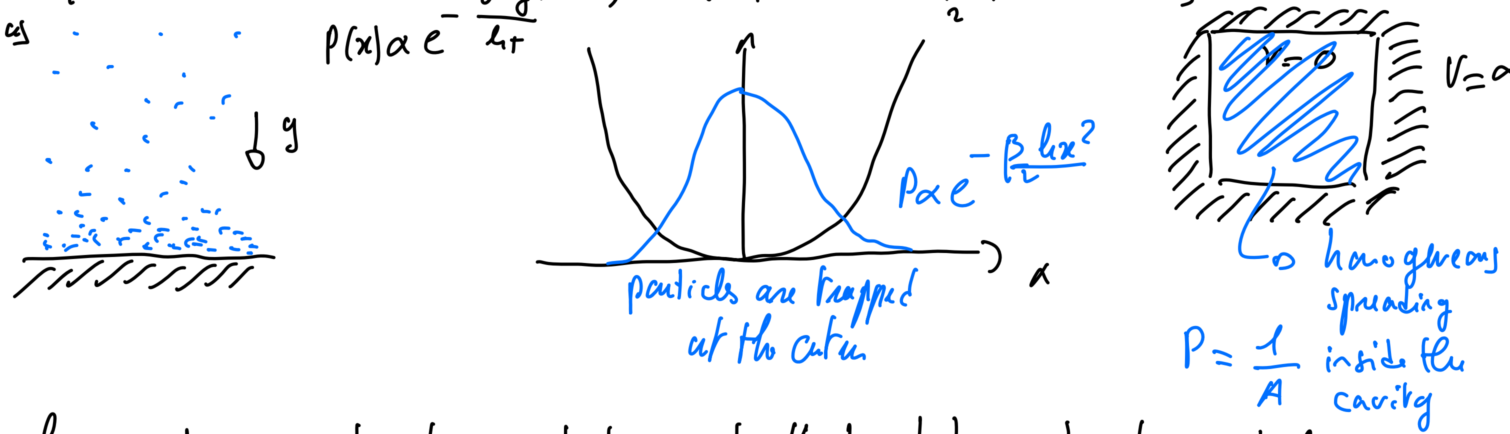
In this sense, the dissipation w_p characterizes the departure from thermal equilibrium of the system and it thus attracted a lot of interest.

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

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

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

<u>Equilibrium</u>:



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.

a) Sedimentation

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

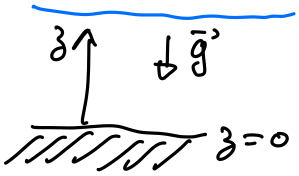
$\dot{\vec{r}} = -v_s \hat{z} + \vec{v}_p$ ($\hat{z}$ unit vector along z-axis)

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

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

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

$z \gg \ell_p$



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

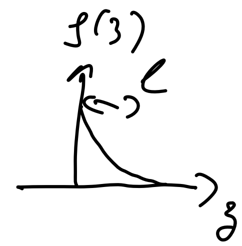
$$\lambda_{2D} = \frac{2\alpha v_s}{v_p^2 - v_s^2}$$

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

Refs: | Tailleur, Cates, PRL 2008
| Cates, Tailleur, EPL 2009 & references therein.
| Solon, Cates, Tailleur, EPJST 2015

Comments:

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



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

$\to$ add translational noise $\dot{\vec{r}} = \vec{v}_p + \vec{v}_s + \sqrt{2D_t}\,\vec{\eta}$
$\hookrightarrow$ regularize a finite sedimentation length.

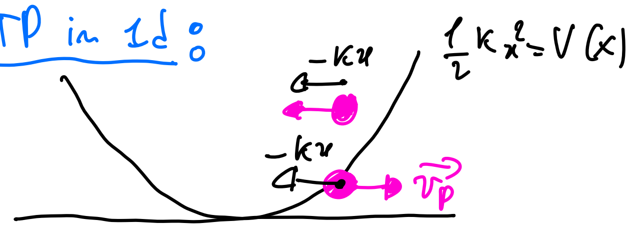
* $v_s \ll |v_p| \Rightarrow \lambda \simeq \dfrac{d\alpha v_s}{v^2} \Rightarrow P \propto e^{-\frac{\mu\delta m g z d\alpha}{v^2}} \equiv e^{-\frac{\delta m g z}{kT_{eff}}}$

$kT_{eff} = \dfrac{v^2}{d\alpha\mu} \Rightarrow$ effective temperature regime

b) Confinement

Harmonic trap $V(x) = \frac{1}{2}kx^2$

RTP in 1d:



$v_R = v_p - kx \qquad \alpha_R = \alpha_L = \alpha$

$v_L = v_p + kx \qquad P(x,\pm) =$ proba to go right/left at x

$$\partial_t P(x,+) = -\partial_x\left[(v_p - kx)P(x,+)\right] - \frac{\alpha}{2}P(x,+) + \frac{\alpha}{2}P(x,-)$$

$$\partial_t P(x,-) = -\partial_x\left[-(v_p + kx)P(x,-)\right] + \frac{\alpha}{2}P(x,+) - \frac{\alpha}{2}P(x,-)$$

Steady-state: $\partial_t P(x,\pm) = 0 \Rightarrow$ compute $P(x) = P(x,+) + P(x,-)$

8

Exact solution: $P(x) = P(0)\left[1 - \left(\frac{kx}{v_p}\right)^2\right]^{\frac{1}{2k\tau} - 1}$ [Tailleur, Cates, PRL 2008]

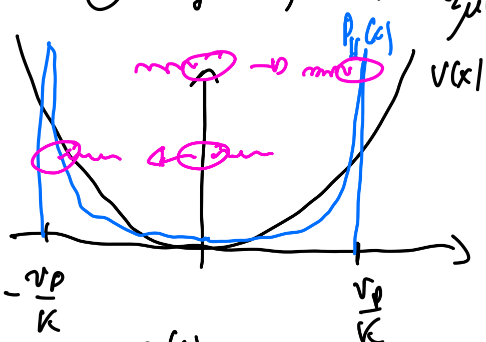
① if $x > \frac{v_p}{k}$, $v_R < 0$; $x < -\frac{v_p}{k}$, $v_L > 0$ } bounded horizon $\left[-\frac{v_p}{k}, \frac{v_p}{k}\right]$ accessible to the particles

② $\tau \to 0$, $P = 0$ if $x \neq 0$ $\Rightarrow$ $P(x) \sim e^{\frac{1}{2\mu k\tau}\ln\left[1 - \left(\frac{\mu k x}{v_p}\right)^2\right]}$

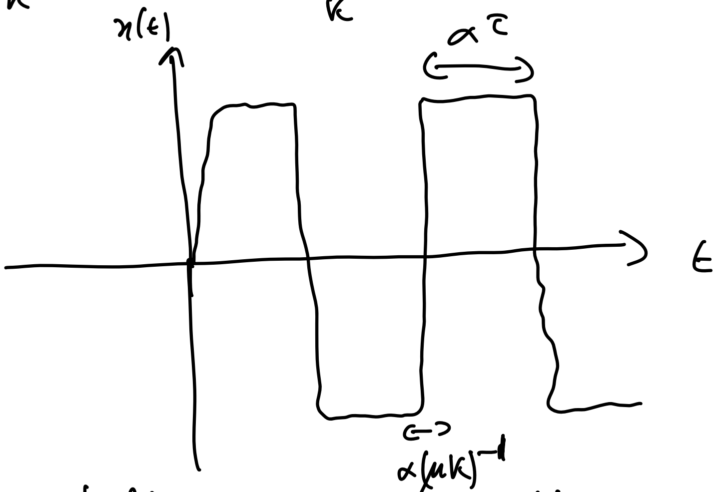
$$\sim e^{-\frac{1}{2\mu k\tau}\cdot\left(\frac{\mu k x}{v_p}\right)^2} = e^{-\frac{\mu k x^2}{2\tau v_p^2}} = e^{-\beta_{eff}\frac{kx^2}{2}}$$

Effective equilibrium with $kT_{eff} = \frac{v_p^2\tau}{\mu} = \frac{D_{eff}}{\mu}$

③ Large τ, $\tau > \frac{1}{2\mu k\tau}$ $\Rightarrow$ $\frac{1}{2\mu k\tau} - 1 < 0$ $P(x)$ diverges as $x \to \pm\frac{v_p}{\mu k}$



$\Rightarrow$ Accumulation at the horizon



$\Rightarrow$ accumulation at $x = \pm\frac{v_p}{k}$

Very different with an equilibrium system $\Rightarrow$ the particle is almost never found at the center of the trap.