2.3) Active Ornstein Uhlenbeck Particles (AOUPs)

So far ABPs and RTPs are such that $P(|\vec{v}|) = \delta(|\vec{v}| - v_0)$

→ since $\dot{\vec{r}} = \underbrace{v_0}_{\text{self propulsion of modulus } v_0} u(\theta) + \dots$

⇒ no fluctuation of the self-propulsion speed.

Sometimes, this is ok ⇒ Janus colloids [Ginot et al, New Journal of Physics 20, 115001 (2018)]

Sometimes not → cells [Sepulveda et al, PLOS Comp. Biol. 9, e1002944 (2013)]

Q: How to model fluctuations of self-propulsion?

Active Ornstein Uhlenbeck particle

$$\dot{\vec{r}} = \underbrace{\vec{v}_p}_{\text{self propulsion}} - \mu \vec{\nabla} V \quad ; \quad \underbrace{\tau \dot{\vec{v}}_p = -\vec{v}_p + \sqrt{2D}\, \vec{\eta}}_{\text{Ornstein-Uhlenbeck process}} \quad (*)$$

$$\dot{\vec{v}}_p = -\frac{\vec{v}_p}{\tau} + \sqrt{\frac{2D}{\tau^2}}\, \vec{\xi}$$

Dynamics of self-propulsion speed (*):

All components v_p^i are independent ⇒ $P(\vec{v}_p) = \prod_i p(v_p^i)$

Fokker-Planck equation $\partial_t p(v_p^i) = \frac{\partial}{\partial v_p^i}\left[\frac{D}{\tau^2}\frac{\partial}{\partial v_{p_i}} + \frac{v_{p_i}}{\tau}\right] p(v_p^i)$

steady-state solution is $p(v_p^i) = \sqrt{\frac{\tau}{2\pi D}}\, e^{-\frac{1}{2}\frac{\tau (v_p^i)^2}{D}}$

All in all $P(\vec{v}_p) = \left(\frac{\tau}{2\pi D}\right)^{d/2} \exp\left[-\frac{1}{2}\frac{\tau \vec{v}_p^{\,2}}{D}\right]$ in dimension d.

Comment: * $\langle \vec{v}_p \rangle = 0$; $\langle \vec{v}_p^{\,2} \rangle = d\,\frac{D}{\tau}$

typical scale of self propulsion speed $\boxed{v_0 = \sqrt{d\,\frac{D}{\tau}}}$

* ABPs, RTPs, AOUPs all have typical speeds ⇒ very different fluctuations

A OUPs is a linear, Gaussian Process

$$P(|v_p|) \propto \underbrace{|v_p|^{d-1}}_{\text{Jacobian } (v_p^i,\dots)\to|v_p|} e^{-\frac{1}{2}\frac{\tau v_p^2}{D}}$$

→ ABPs and RTPs are strongly non-Gaussian $P(|v_p|) = \delta(|v_p|-v_0)$

END 1st lecture

3) Some insight on the dynamics

3.1) 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:

$$\frac{d}{dt}\langle \vec{u}(\theta(t))\cdot\vec{u}(0)\rangle = \frac{d}{dt}\langle \vec{u}(\theta(t))\rangle\cdot\vec{u}(0)$$

$$= \frac{d}{dt}\int d^2\vec{r}\,d\theta\; P(\vec{r},\theta,t)\,\vec{u}(\theta)\cdot\vec{u}(0)$$

$$= \int d^2\vec{r}\,d\theta\;\frac{dP}{dt}\;\vec{u}(\theta)\cdot\vec{u}(0)$$

$$\frac{dP}{dt} = \underbrace{-\vec{\nabla}_{\vec{r}}\cdot\left[v_p\,\vec{u}(\theta)\,P\right]}_{\int d^2\vec{r}\,[\dots]=0 \text{ since } P\xrightarrow[\vec{r}\to\infty]{}0} - \alpha P + \frac{\alpha}{2\pi}\rho(\vec{r})\;;\quad \rho(\vec{r}) = \int d\theta\, P(\vec{r},\theta)$$

$$\hookrightarrow \int d\theta\,\rho(\vec{r})\,\vec{u}(\theta) = 0 \quad \text{(symmetry)}$$

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

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

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

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

Active Brownian Particles

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

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

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

$$\frac{d}{dt}\langle \vec{u} \rangle \overset{\text{Itō}}{=} 0 - D_r\langle \vec{u} \rangle \quad \text{since } \langle \vec{u}^{\perp}(\theta(t))\,\xi(t) \rangle \overset{\text{Itō}}{=} \langle \vec{u}^{\perp}(\theta(t)) \rangle \times \underbrace{\langle \xi(t) \rangle}_{=0}$$

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

then $\tau = \frac{1}{D_r}$ ([rotational diffusivity] $= T^{-1}$)

d dimension: Same path as RTPs & $\Delta_{\vec{u}}\vec{u} = -(d-1)\vec{u}$

leads to $\tau = \frac{1}{(d-1)D_r}$

Active Ornstein Uhlenbeck particles:

$$\partial_t \underbrace{\langle v_p^i(t)\, v_p^i(0) \rangle}_{f(t)} = \langle \partial_t v_p^i(t)\, v_p^i(0) \rangle = -\frac{1}{\tau} \underbrace{\langle v_p^i(t)\, v_p^i(0) \rangle}_{f(t)} + \frac{\sqrt{2D}}{\tau} \underbrace{\langle \eta^i(t)\, v_p^i(0) \rangle}_{=0}$$

$$\Rightarrow \langle v_p^i(t)\, v_p^i(0) \rangle = \underbrace{\langle v_p^i(0)^2 \rangle}_{\frac{D}{\tau}} e^{-\frac{t}{\tau}}$$

$$\partial_t f(t) = -\frac{1}{\tau} f(t) \Rightarrow f(t) = f(0)\, e^{-\frac{t}{\tau}}$$

$$\langle \vec{v}_p(t) \cdot \vec{v}_p(0) \rangle = \frac{dD}{\tau} e^{-\frac{t}{\tau}} = v_0^2\, e^{-\frac{t}{\tau}}$$

Again, the self propulsion has a finite persistence time τ.

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

$\tau \dot{\vec{v}}_p = -\vec{v}_p + \sqrt{2D}\,\vec{\eta}$ for AOUPs.

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

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

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

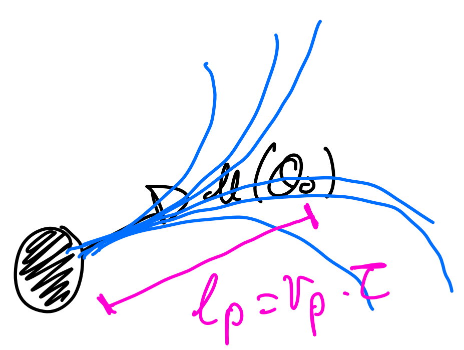
$$= \langle \vec{v}_p(0)\rangle \tau (1 - e^{-t/\tau})$$

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

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

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 $t=0$.



AOUPs $\left\langle (\vec{r}(t) - \vec{r}(0)) \cdot \frac{\vec{v}_p(0)}{|v_p(0)|} \right\rangle \underset{t\to\infty}{\sim} \langle |\vec{v}_p(0)| \rangle \cdot \tau$

$$\left[\int_0^\infty dx \; x e^{-\frac{x^2}{2\sigma}} = \left[-\sigma e^{-\frac{x^2}{2\sigma}} \right]_0^\infty = \sigma \right.$$

$$\left. \int_{-\infty}^{+\infty} dx \frac{|x| \; e^{-\frac{x^2}{2\sigma}}}{\sqrt{2\pi\sigma}} = \frac{2\sigma}{\sqrt{2\pi\sigma}} = \sqrt{\frac{2\sigma}{\pi}} \right]$$

$$\ell_p = \sqrt{\frac{2D}{\pi\tau}} \cdot \tau = \sqrt{\frac{2D\tau}{\pi}}$$

3.3) Large-scale diffusive regime

3.3.1) Diffusion in uniform environment

ABPs, RTPs and AOUPs all undergo different types of persistent random walks. Let's consider a long trajectory

$$\vec{r}(t) = \int_0^t ds \; \dot{\vec{r}}(s) = \sum_{k=0}^{N-1} \int_{k\Delta t}^{(k+1)\Delta t} ds \; \dot{\vec{r}}(s)$$

when $N = \frac{t}{\Delta t}$. If $\Delta t \gg \tau$; $\Delta \vec{r}_k = \int_{k\Delta t}^{(k+1)\Delta t} ds \; \dot{\vec{r}}(s)$ are independent. Because $\dot{\vec{r}}(s) = \vec{v}_p$, the RV $\Delta \vec{r}_k$ have finite moments and CLT apply to large-scale motion should be diffusive.

Green-Kubo:

ABPs & RTPs: $\langle \vec{v}_p(t) \cdot \vec{v}_p(0) \rangle = v_p^2 \, e^{-t/\tau}$

$$D = \frac{1}{d} \int_0^\infty dt \, v_p^2 \, e^{-t/\tau} = \frac{v_p^2 \tau}{d}$$

$$D_{ABP} = \frac{v_p^2}{d(d-1)D_r} \qquad \& \qquad D_{RTP} = \frac{v_p^2}{\alpha d}$$

AOUPs: $\langle \vec{v}_p(t) \cdot \vec{v}_p(0) \rangle = \langle v(0)^2 \rangle \, e^{-t/\tau}$; $\langle v(0)^2 \rangle = \frac{dD}{\tau}$

$$D_{AOUPs} = \frac{D}{\tau} \int_0^\infty dt \, e^{-t/\tau} = D \qquad \text{(hence the name)}$$

Comment: some interesting differences

* Take a RW of steps l_p, made every $\tau \Rightarrow D = \frac{1}{d} \frac{l_p^2}{\tau}$
  applies for ABPs & RTPs
  not for AOUPs because of the fluctuations of v_p

* $D_{ABP,RTP} \propto \frac{1}{d} \Rightarrow$ self-propulsion along 1 direction $\vec{u}(0)$

  $D_{AOUPs} \underset{d}{\propto} O(1) \Rightarrow$ ——— along all direction

  (else, take $D \sim \frac{1}{d}$)

Part below not done in class $\Rightarrow$ MIPS lectures

3.3.2) Diffusive limit with inhomogeneous self-propulsion speed

RTPs in 1D Diffusive limit: $\alpha_R = \alpha_L = \alpha$; $v_R = v_L = v$; $t \gg 1/\alpha$

$$\begin{cases} \partial_t R(x,t) = -v\,\partial_x [R(x,t)] - \alpha R(x,t) + \alpha L(x,t) \\ \partial_t L(x,t) = v\,\partial_x [L(x,t)] + \alpha R(x,t) - \alpha L(x,t) \end{cases}$$

$\rho = R + L$ local probability density

$$\boxed{\partial_t \rho = (1)+(2) = -\partial_x [J_R - J_L] = -\partial_x [v(R-L)] = -\partial_x \cdot J}\ ; \quad J = vR - vL \quad (*)$$

what is the value of J?

$$v(1) - v(2) = \partial_t J = -v\,\partial_x [v(R+L)] - \alpha v R + \alpha v L$$

$$\boxed{\partial_t J = -v\,\partial_x [\rho \cdot v] - \alpha J} \qquad (**)$$

$$(**) \Rightarrow \quad J_p = J_0 e^{-\alpha t} + e^{-\alpha t} \int_0^t ds\, e^{\alpha s} (-v\,\partial_x(\rho v))$$

ρ is a conserved field $\Rightarrow$ on time-scale $\sim \frac{1}{\alpha}$ it barely evolves

$$J = J_0 e^{-\alpha t} + \int_0^t ds\, \underbrace{e^{-\alpha(t-s)}}_{\simeq 0 \text{ if } t-s \gg 1/\alpha} (-v\,\partial_x(\rho v))$$

$$\simeq \underbrace{J_0 e^{-\alpha t}}_{\simeq 0\ t \gg 1/\alpha} - [v\,\partial_x(\rho v)] \underbrace{\int_0^t ds\, e^{-\alpha(t-s)}}_{\simeq 1/\alpha\ t \gg 1/\alpha} \simeq -\frac{v}{\alpha}\partial_x(\rho v)$$

Injecting this in (*) leads to $\boxed{\partial_t \rho = \partial_x \left[\frac{v}{\alpha} \partial_x (\rho v) \right]}$ (***)

(***) is a diffusion-drift approximation of the microscopic run and tumble dynamics.

The same in 2D, and for ABPs: Cates, Tailleur, EPL 101, 20010 (2013)
The — for AOUPs: Martin et al, PRE 103, 032607 (2021)

* If v is a constant $\Rightarrow \partial_t \rho = \frac{v^2}{\alpha} \partial_{xx} \rho \Rightarrow D = \frac{v^2}{\alpha}$ and we recover the result in uniform space.

* If $v(x)$ non-constant $\Rightarrow \rho = \frac{K}{v(x)}$ is a steady-state solution if $\int_{\mathbb{R}} dx \frac{1}{v(x)} < \infty$

$\Rightarrow$ Active particles are more likely to be found where they go slower!

3.3.3) From micro to macro

ABPs in 2D

$$\dot{\vec{r}} = v_0 \vec{u}(\theta) + \sqrt{2D_t}\, \vec{\eta} \; ; \quad \dot{\theta} = \sqrt{2D_r}\, \xi(t)$$

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

The mean-square-displacement

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

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

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

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

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

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

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

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

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

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

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

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

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

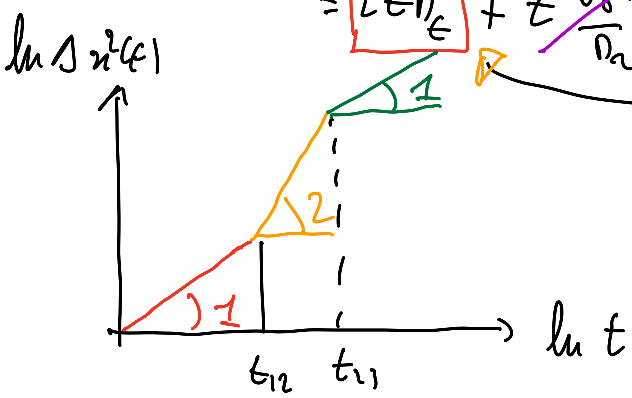
$$= 2t\left[D_t + \frac{v_0^2}{2D_r}\right] + \frac{v_0^2}{2D_r}\left\{\frac{e^{-D_r t}-1}{D_r} - \frac{1-e^{-D_r t}}{D_r}\right\}$$

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

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

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

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



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 once again $\Delta x^2 \sim D_{eff}\, t$

t_{12} and t_{23} may be hard to observe simultaneously

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

$\rightarrow \theta_0$

$\rightarrow$ the realisations of $\{\xi(t), \eta_x(t), \eta_y(t)\}$.

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

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

$$t_{23} = \frac{2}{D_r} = 2\tau_r$$

2c

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) Non-Boltzmann Steady States

In equilibrium, $V(x) \Rightarrow$ Boltzmann weight $P(x) = \frac{1}{Z} e^{-\beta V(x)}$

N non-interacting particles $\rho(x) = \sum_{i=1}^{N} \delta(x - x_i)$

$$P[\rho] \propto e^{-\beta \hat{f}[\rho]} \qquad \hat{f} = \int dx \underbrace{V(x)\rho(x)}_{\text{density of NRG}} + \underbrace{kT \rho(x)(\ln \rho(x) - 1)}_{-T \times \text{density of entropy}}$$

Proof: $\dot{x}_i = -\mu V'(x_i) + \sqrt{2\mu kT}\, \eta_i$

$$\frac{d\rho}{dt} = \sum_{i=1}^{N} -\dot{x}_i \delta'(x - x_i) + \mu kT \delta''(x - x_i)$$

$$= \sum_{i=1}^{N} -\partial_x \left[\left(-\mu V'(x_i) + \sqrt{2\mu kT}\, \eta_i\right) \delta(x - x_i) \right] + \partial_x^2 \left[\mu kT \delta(x - x_i) \right]$$

commute

$$= \sum_{i=1}^{N} \partial_x \left[\mu V'(x) \delta(x - x_i) - \sqrt{2\mu kT}\, \eta_i \delta(x - x_i) + \mu kT \partial_x \delta(x - x_i) \right]$$

$$= \partial_x \left[\mu V'(x) \sum_i \delta(x - x_i) + \mu kT \partial_x \sum_{i=1}^{N} \delta(x - x_i) - \sum_{i=1}^{N} \sqrt{2\mu kT}\, \eta_i \delta(x - x_i) \right]$$

$$\partial_t \rho(x,t) = \partial_x \left[\mu V'(x) \rho(x) + \mu kT \partial_x \rho(x) + \Lambda(x,t) \right] \qquad (*)$$

where $\Lambda(x,t) = \sum_{i=1}^{N} \sqrt{2\mu kT}\, \eta_i \delta(x - x_i)$

For given x_i,

$$\langle \eta(x,t)\eta(x',t')\rangle = \sum_{i,j} 2\mu k_B T\, \delta(x-x_i)\,\delta(x'-x_j)\quad \delta_{ij}\,\delta(t-t')$$

$$= 2\mu k_B T \sum_{i=1}^{N} \underbrace{\delta(x-x_i)\,\delta(x'-x_i)}_{\delta(x-x_i)\,\delta(x'-x)}\,\delta(t-t')$$

$$= 2\mu k_B T\, \delta(t-t')\,\delta(x'-x) \sum_{i=1}^{N} \delta(x-x_i)$$

$$\langle \eta(x,t)\eta(x',t')\rangle = 2\mu k_B T\, \rho(x,t)\,\delta(t-t')\,\delta(x-x')$$

$$(*) \Leftrightarrow \quad \partial_t \rho = \partial_x \left[\mu V'(x)\rho(x) + \mu k_B T\, \partial_x \rho(x) + \sqrt{2\mu k_B T \rho(x)}\;\xi(x,t)\right]$$

when $\langle \xi(x,t)\,\xi(x',t')\rangle = \delta(x-x')\,\delta(t-t')$

Functional Fokker-Planck equation

[Solon et al, EPJST 224 1231-1262 (2015)]

$$\frac{d}{dt} P[\{\rho\},t] = \int dx\, \frac{\delta}{\delta\rho(x)}\, \partial_x \underbrace{\left[-\mu V'(x)\rho(x) - \mu k_B T\, \partial_x \rho(x) - \mu k_B T \rho(x)\left(\partial_x \frac{\delta}{\delta\rho(x)}\right)\right]}_{J[\rho]} P$$

Ansatz $P[\rho] = e^{-\beta \hat{f}[\rho]}$

$$J = 0 \Leftrightarrow \quad -\mu V'\rho - \mu k_B T\, \partial_x \rho + \mu \quad \rho\, \partial_x \frac{\delta \hat{f}}{\delta \rho} = 0$$

$$\Leftrightarrow \quad \partial_x \frac{\delta \hat{f}}{\delta \rho} = V'(x) + k_B T\, \partial_x \ln \rho(x)$$

$$\Leftrightarrow \quad \frac{\delta \hat{f}}{\delta \rho} = V(x) + k_B T \ln \rho(x) \Rightarrow$$

$$\mathcal{F}[\rho] = \int dx \; \rho(x) V(x) + k_B T \rho(x)[\ln \rho(x) - 1]$$

$\mathcal{F}[\rho]$ Landau free energy of the macro state $\rho(x)$

$\Rightarrow$ steady-state controlled by balance between entropy and energy $\Rightarrow$ relative weight set by T.

$\Rightarrow$ lot of intuition on equilibrium systems

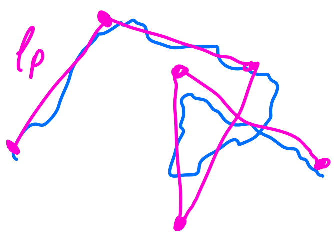
$\Rightarrow$ What about active ones?

4.1) The equilibrium limit

Active particles are characterized by a persistence length ℓ_p and a persistence time τ.

Naive picture: Make steps in a random direction every ℓ/τ time units.

$\Rightarrow$ passive random walk picture!



Exercise: write down the master equation of the particle position $\Rightarrow$ compute the diffusivity.

$$[D] = L^2 . T^{-1} \Rightarrow D \propto \frac{\ell_p^2}{\tau} \times \frac{1}{d}$$

$$\boxed{\text{diffusivity} : \lim_{t\to\infty} \frac{1}{t} \frac{\langle r^2(t)\rangle}{2d} \qquad \langle r^2 \rangle \sim 2dDt}$$

e.g. ABP, $\tau = \frac{1}{D_r}$, $\ell_p = \frac{v}{D_r} \Rightarrow D = \frac{v^2}{d D_r}$ ✓

RTP, $\tau = \frac{1}{\alpha}$, $\ell_p = \frac{v}{\alpha} \Rightarrow D = \frac{v^2}{d\alpha}$ ✓

Q: Does this mean that large-scale active matter is equivalent to "hot" colloid suspensions in equilibrium.

→ in general, no.

→ but there are interesting exceptions.

The small τ regime at fixed D:

In the limit $\tau \to 0$, D constant, active dynamics become fully equivalent to colloidal dynamics at an effective temperature $kT_{eff} = \frac{D}{\mu}$ where D is the large-scale diffusivity of the active particle and μ is their mobility.

proof for AOUPs:

$$\dot{\vec{r}} = -\mu \vec{\nabla} V(\vec{r}) + \vec{v} \; ; \; \tau \dot{\vec{v}} = -\vec{v} + \sqrt{2D}\,\vec{\xi}$$

$$\tau \to 0 \Rightarrow \vec{v} = \sqrt{2D}\,\vec{\xi} \; ; \; \dot{\vec{r}} = -\mu \vec{\nabla} V(\vec{r}) + \sqrt{2D}\,\vec{\xi}$$

$$P_s(\vec{r}) = Z^{-1} \exp\left[-\frac{\mu}{D} V(\vec{r})\right]$$

$$\Rightarrow kT_{eff} = \frac{D}{\mu}$$

Interesting Q: how does P_s depart from Boltzmann as τ increases? ⇒ O'Byrne et al, Nat. Rev. Phys. 2022 arXiv: 2104.03030

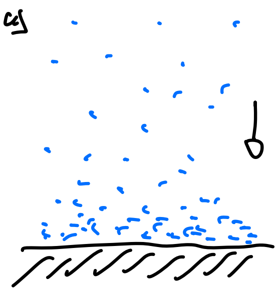
4.2) External potentials

The breakdown of FDT means that the steady-state distribution need not be the Boltzmann weight, outside the $\tau = 0$ limit.

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

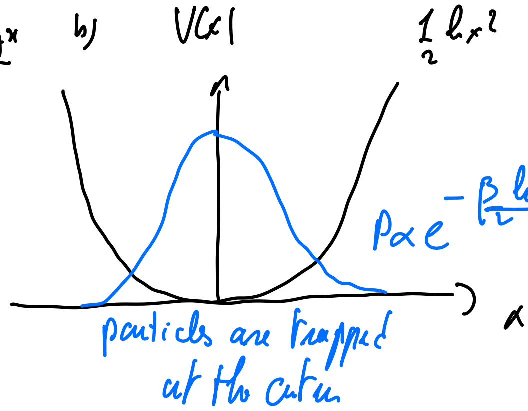
Equilibrium:

a)

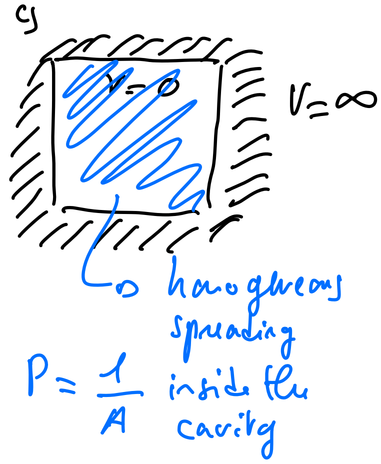


$P(x) \propto e^{-\frac{\delta m g x}{k_T}}$

b)



c)



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.

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

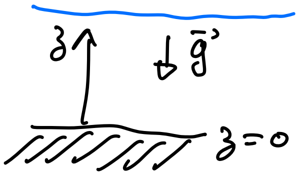
$\vec{v}_s$ Stokes sedimentation speed $v_s = \mu \delta m g = -\partial_z V_{gravity}(z) \times \mu$

speed at which particle falls at $T=0$

$\vec{v}_p$ self-propulsion speed

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

$z \gg \ell_p$



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

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

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