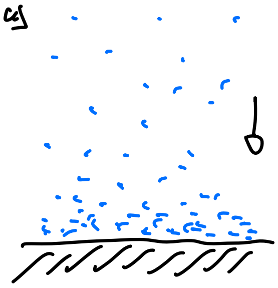
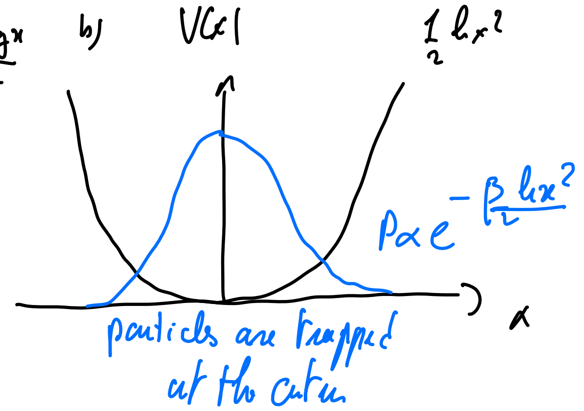
Equilibrium:

a)

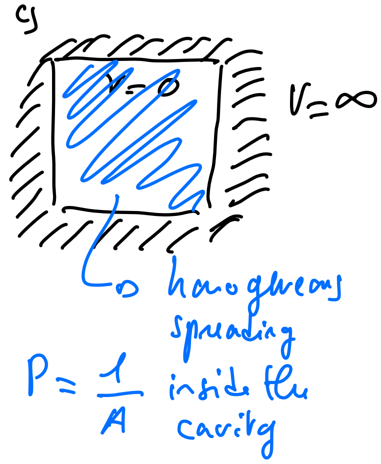


$P(x) \propto e^{-\frac{\delta m g x}{k_T}}$

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

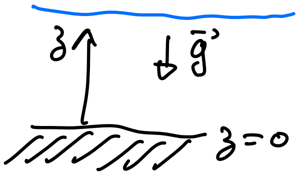
A bunch of exact results and some experiments on the sedimentation of active particles.

$\vec{r} = -v_s \hat{z} + \vec{v}_p$ ($\hat{z}$ 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: $P_s(z) = \frac{1}{Z} e^{-\lambda z}$ ⇒ 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

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

λ_{3D} → 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
Solon, Cates, Tailleur, EPJST 2015

Comments:

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

→ 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.

→ add translational noise $\dot{\vec{r}} = \vec{v}_p + \vec{v}_s + \sqrt{2D_t}\,\vec{\eta}$

↳ regularize a finite sedimentation length.

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

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

*** AOUPs** $P_s(z) = \frac{1}{Z} e^{-\lambda z}$; $\lambda = \frac{v_s}{D}$ $\forall v_s \Rightarrow$ always have an equilibrium regime.

[Szamel, 2014, PRE]

*** ABPs** No explicit solution, implicit one in the form of Mathieu functions.
[Solon, Cates, Tailleur, EPJST 2015]

Take-home message:
* qualitatively similar to equilibrium
* see differences between the models: ABP & RTP → gravitational collapse.

b) Confinement

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

AOUPs [Szamel, 2014, PRE] $P(x) = \frac{1}{Z} e^{-\beta_{eff} \frac{k x^2}{2}}$

where $k_B T_{eff} = (\beta_{eff})^{-1} = \frac{D}{\mu} \times \underbrace{(1+\mu\tau k)^{-1}}_{= \sum_n (-1)^n (\mu\tau k)^n}$ ⇒ correction to the thermal equilibrium regime as $\tau \to 0$

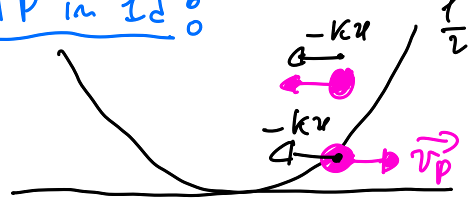
Stokes-Einstein

Qualitatively → always a Gaussian as in equilibrium

→ "Temperature" that depends on K ⇒ unlike equilibrium

The control parameter that controls the distance to the $\tau=0$ limit is $\frac{\tau}{\tau_c}$ where $\tau_c = \frac{1}{\mu k}$ is the relaxation time of the potential.

RTP in 1d :



$\frac{1}{2} k x^2 = V(x)$

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

$v_L = v_p + kx$

] Solve the steady state

$\partial_t R(x,t) = \partial_t L(x,t) = 0$ ⇒ compute $\rho(x,t) = R(x,t) + L(x,t)$

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

① if $x > \frac{v_p}{k}$ $v_R < 0$

$x < -\frac{v_p}{k}$ $v_L > 0$

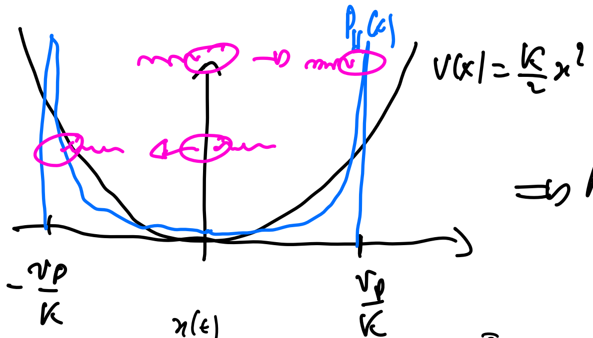
} bounded horizon $\left[-\frac{v_p}{k}, \frac{v_p}{k}\right]$ accessible to the particle

② $\tau \to 0$, P_{1d} dominated by $x \simeq 0$ ⇒ $P_{1d}(x) \sim e^{\frac{1}{2\mu k \tau} \ln\left[1 - \left(\frac{\mu k x}{v_p}\right)^2\right]}$

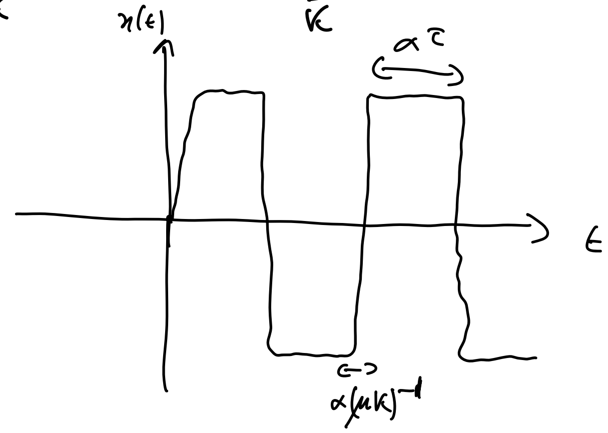
$\sim e^{-\frac{1}{2\mu k \tau} \cdot \left(\frac{\mu k x}{v_p}\right)^2} = e^{-\frac{\mu k x^2}{2 \tau v_p^2}} = e^{-\beta_{eff} \frac{k x^2}{2}}$

Effective equilibrium with $k_B T_{eff} = \frac{v_p^2 \tau}{\mu} = \frac{D_H}{\mu}$

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



$\Rightarrow$ Accumulation at the horizon



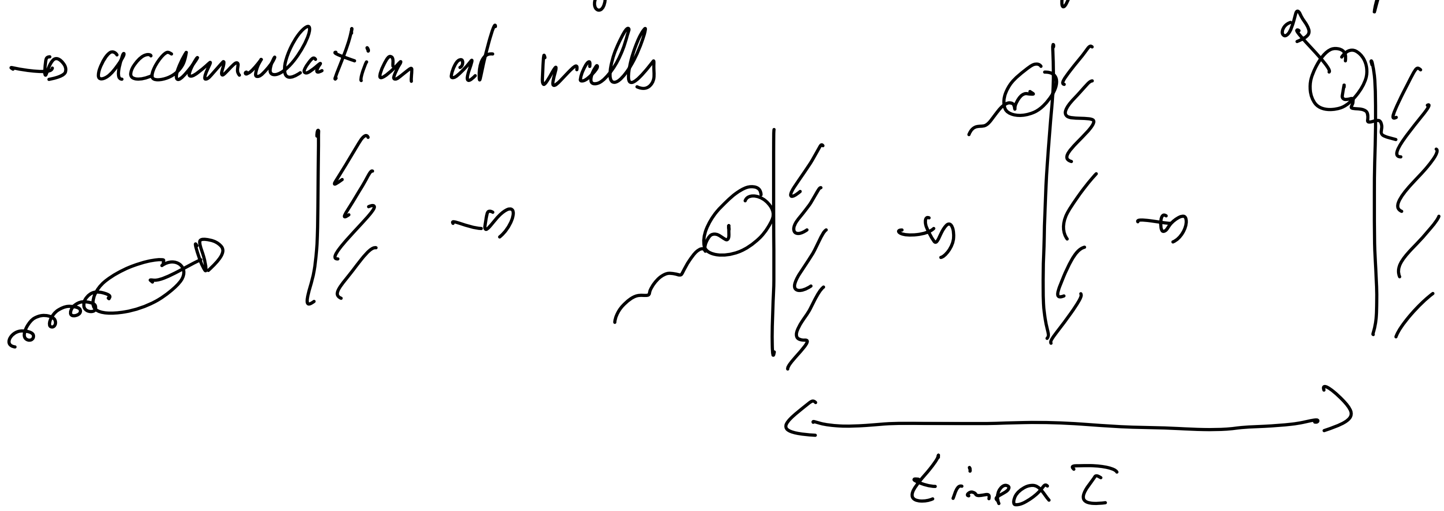
$\Rightarrow$ accumulation at $x = \pm \frac{v_p}{k}$

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

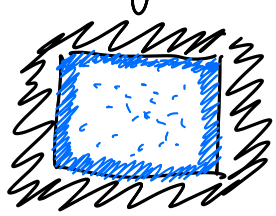
c) active particles and walls

This result is much more general than the case of harmonic traps.

$\rightarrow$ accumulation at walls



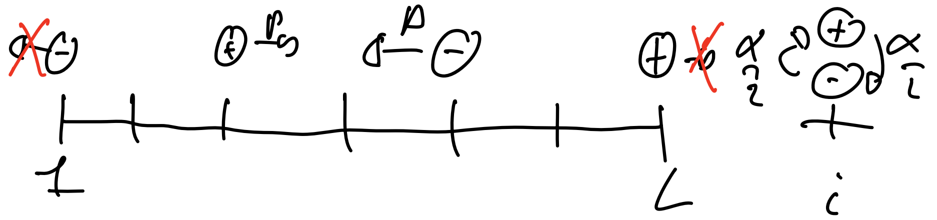
The persistence of active particles make them accumulate at walls



$v_p \tau \gg L \Rightarrow$ all particles at the wall

[Elgeti, Gompper, EPL 2009]

1d lattice model:



$$\begin{cases} \partial_t P_i^+ = p\, P_{i-1}^+ - p\, P_i^+ - \frac{\alpha}{2} P_i^+ + \frac{\alpha}{2} P_i^- & i = 2, \dots, L-1 \\ \partial_t P_i^- = p\, P_{i+1}^- - p\, P_i^- + \frac{\alpha}{2} P_i^+ - \frac{\alpha}{2} P_i^- & i = 2, \dots, L-1 \end{cases}$$

$$\partial_t P_L^+ = p P_{L-1}^+ - \frac{\alpha}{2} P_L^+ + \frac{\alpha}{2} P_L^- \; ; \; \partial_t P_L^- = -p P_L^- + \frac{\alpha}{2} P_L^+ - \frac{\alpha}{2} P_L^-$$

$$\partial_t P_1^- = p\, P_2^- + \frac{\alpha}{2} P_2^+ - \frac{\alpha}{2} P_2^- \; ; \; \partial_t P_1^+ = -p P_1^+ - \frac{\alpha}{2} P_1^+ + \frac{\alpha}{2} P_1^-$$

$$\rho_i = P_i^+ + P_i^- \Rightarrow \partial_t \rho_i = -p\,[\underbrace{P_i^+ - P_{i+1}^-}_{J_{i,i+1}}] + p\,[P_{i-1}^+ - P_i^-] = -p\,[J_{i,i+1} - J_{i-1,i}]$$

$$J_{L,L+1} = J_{0,1} = 0$$

steady-state: $\partial_t \rho_i = 0 \Rightarrow J_{i,i+1} = J_{i-1,i} = 0 \Rightarrow P_i^+ = P_{i+1}^-$ $\quad i \in [1, L-1]$

$2 \le i \le L-1$ $\quad \partial_t (P_i^+ - P_i^-) = p\,[\underbrace{P_{i-1}^+}_{=P_i^-} - \underbrace{P_{i+1}^-}_{=P_i^+} + P_i^- - P_i^+] - \alpha\,(P_i^+ - P_i^-)$

$$= 2p\,[P_i^- - P_i^+] - \alpha\,(P_i^+ - P_i^-) \Rightarrow P_i^+ = P_i^- = \rho_b$$

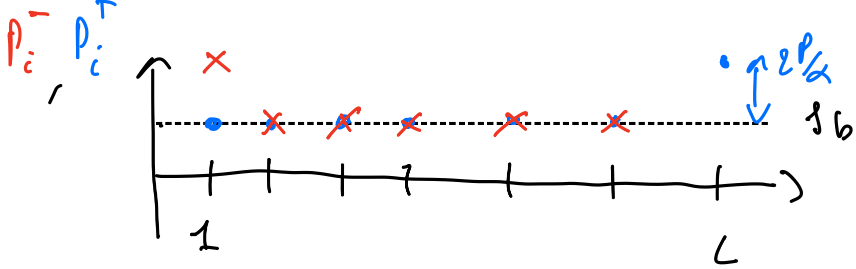
$\partial_t (P_1^+ - P_1^-) = p\,[-P_2^- - P_1^+] - \alpha\,(P_1^+ - P_1^-)$ $\quad$ but $P_2^- = P_1^+$

$$= \alpha P_1^- - (2p + \alpha) P_1^+$$

Steady-state $\quad P_1^- = \frac{2p+\alpha}{\alpha} P_1^+ = \left(1 + 2\frac{p}{\alpha}\right) \rho_b$

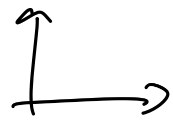
$$\partial_t (P_L^+ - P_L^-) = p\,(P_{L-1}^+ + P_L^-) + \alpha (P_L^- - P_L^+) = (2p+\alpha) P_L^- + \alpha P_L^+$$

Steady-state: $P_L^+ = \left(1 + 2\frac{p}{\alpha}\right) P_L^- = \left(1 + 2\frac{p}{\alpha}\right) \rho_b$



$$\frac{P}{\alpha} = P\tau \xrightarrow[\tau\to 0]{} 0$$

but $P\tau \xrightarrow[\tau\to\infty]{} \infty$



$$\rho_i = \frac{N}{2}\left(\delta_{i,1} + \delta_{i,L}\right)$$

$P(x)$ is then <u>very</u> different from $e^{-\beta V(x)}$

[Elgeti, Gompper, EPL 2009, 2013]

Take home message

① Universal equilibrium regime at $\tau = 0$, D constant
effective temperature : $kT_{eff} = \frac{D}{\mu}$
when D is the large scale diffusivity of the particle.

② Outside $\tau = 0 \Rightarrow$ no universality
AOUPs $\neq$ RTP, ABP

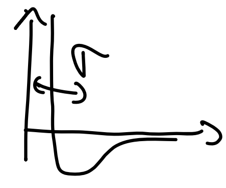
③ Large $\tau \Rightarrow$ strong non-equilibrium effects
. accumulation at walls
. gravitational collapse
. non-monotonous $P(x)$ in traps.

Chapter 2: Motility-Induced Phase Separation

I/ Introduction and phenomenology

I.1/ Passive particles

$\dot{\vec{r}}_i = -\vec{\nabla} V + \sqrt{2D_t}\,\vec{\eta}_i$; Lennard Jones $V = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$



A similar computation to what was done in Chapter I leads to:

$$\rho(\vec{r}) = \sum_i \delta(\vec{r}-\vec{r}_i) \Rightarrow \dot{\rho} = \vec{\nabla}\left[M\nabla\mu + \sqrt{2M}\,\vec{\Lambda}\right]$$

where $M = \rho D_t$ and $\mu(\vec{r}) = \frac{\delta \mathcal{F}}{\delta \rho(\vec{r})}$ with

$$\mathcal{F} = kT\int dx\,(\rho\ln\rho - 1) + \int d^d r\, d^d r'\, \rho(\vec{r})V(\vec{r}-\vec{r}\,')\rho(\vec{r}\,')$$

Steady-state: $P[\rho] \propto e^{-\beta\mathcal{F}[\rho]}$

Most probable ρ minimizes $\mathcal{F}[\rho]$

* Entropy of profile $\rho(\vec{r})$: $S = -k\int d^d r\, \rho(r)(\ln(\rho)-1)$

volume V

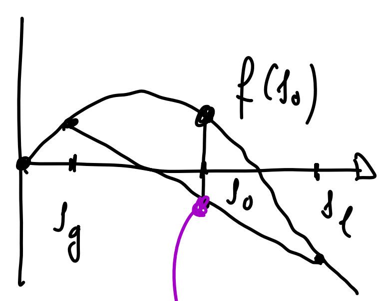
$\rho_H = \rho_0$ vs $\rho_{PS} = \rho_g$ in fraction α, ρ_ℓ in fraction $(1-\alpha)$

$S[\rho_H] = -kVf(\rho_0)$

$S[\rho_{PS}] = -kV[\alpha f(\rho_g) + (1-\alpha) f(\rho_\ell)]$

$f(x) = -x(\ln x - 1)$ concave

$\Rightarrow$ maximal for homogeneous system



$\alpha f_g + (1-\alpha) f_\ell$

* Energy $\quad U = \int d^d\vec{r}\, d\vec{r}\,' \rho(\vec{r})\, V(\vec{r}-\vec{r}\,')\, \rho(\vec{r}\,')$

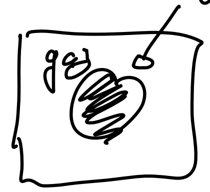
If V attractive ⇒ favors cohesion

* Balance Energy vs Entropy

Large T ⇒ S wins ⇒ homogeneous

Low T ⇒ U — ⇒ liquid-gas phase transition

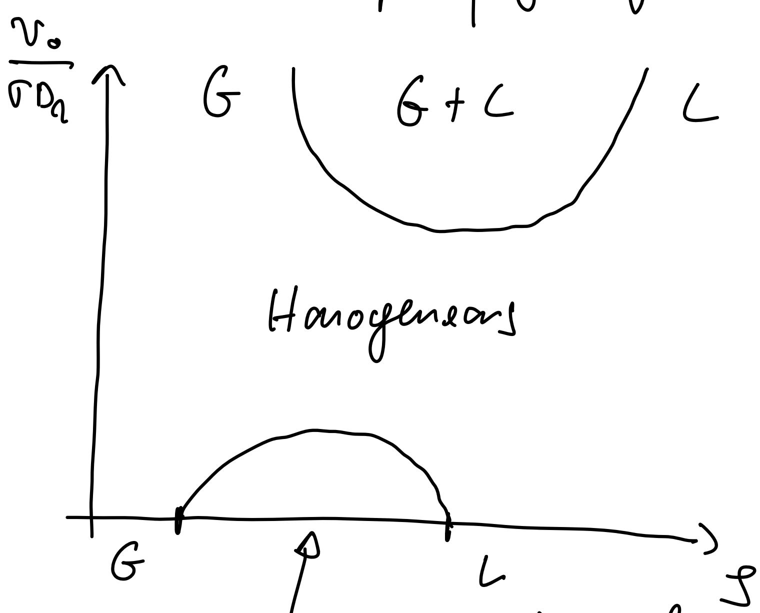
$\int \rho_0 = N$ fixed ⇒ phase coexistence



I.2) Self-propulsion & LJ interactions

$$\begin{cases} \dot{\vec{r}} = -\vec{\nabla} V + v_0\, \vec{u}(\theta) + \sqrt{2D_t}\, \vec{\xi} \\ \dot{\theta} = \sqrt{2D_r}\, \zeta \end{cases} \Rightarrow \text{effect of } v_0\,?$$

Small v_0 helps fighting attractive tail ⇒ vaporise the liquid

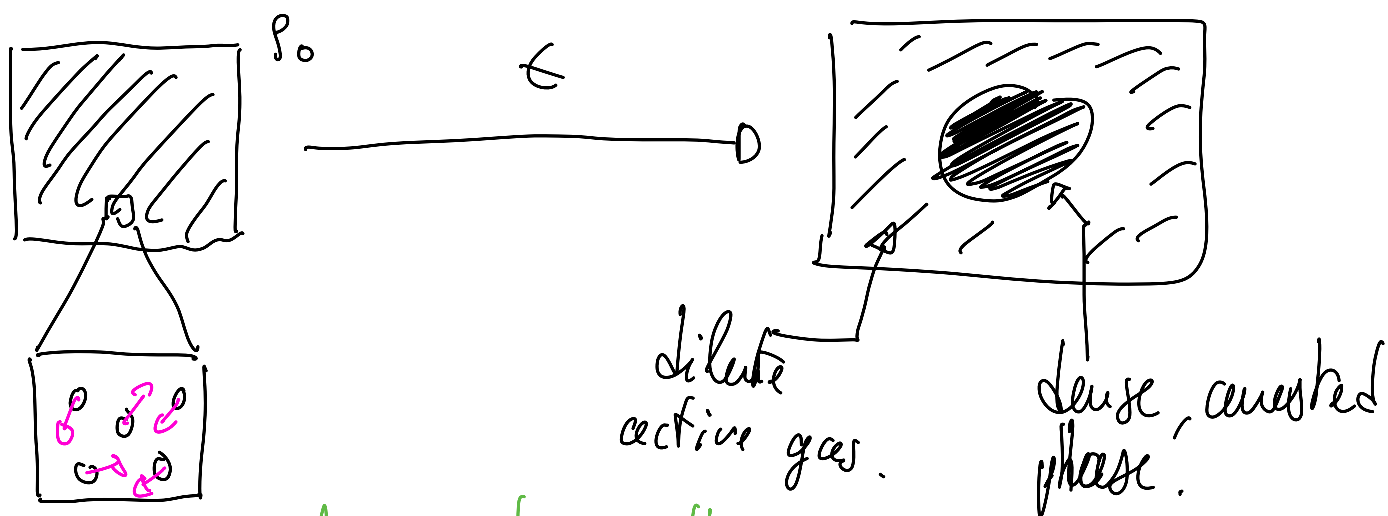


Large v_0 ⇒ surprising reentrance due to motility-induced phase separation

equilibrium liquid-gas phase separation

I.3) Phenomenology & systems

MIPS: Phase transition through which an active system undergoes a phase separation resembling liquid-gas phase separation in the absence of attractive forces.



Very general in active matter:

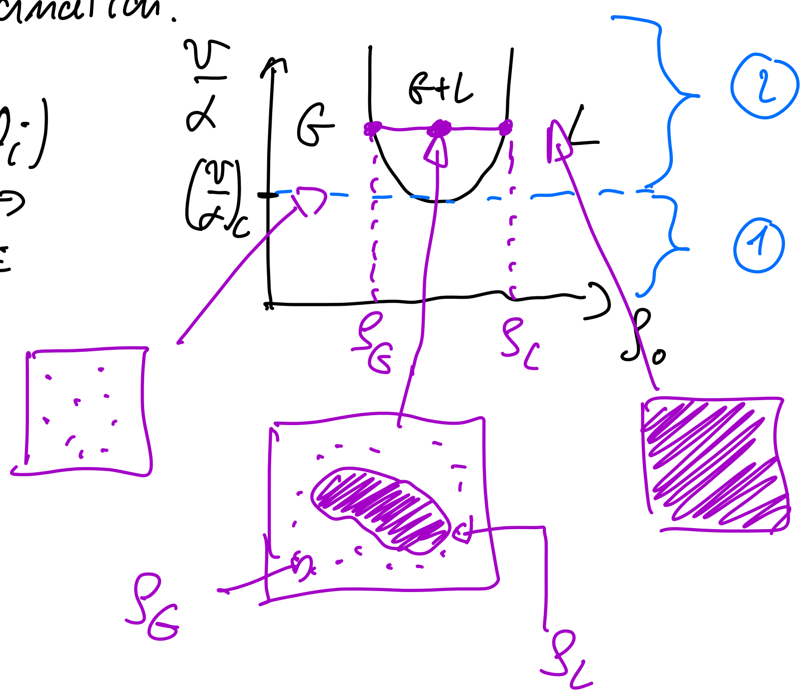
* RTPs [Tailleur, Cates, PRL 101, 218103, (2008)]

on lattice [Thompson et al., J. Stat. Mech. P02029, (2011)]

⇒ quorum-sensing information.

$$\dot{\vec{r}}_i = v(\vec{r}_i, [\rho])\, \vec{u}(\theta_i)$$

$$\theta_i \xrightarrow{\alpha} \theta_i' \qquad + \sqrt{2D_t}\, \vec{\eta}_i$$



In region (1), the translational noise is strong enough to enforce a homogeneous system.

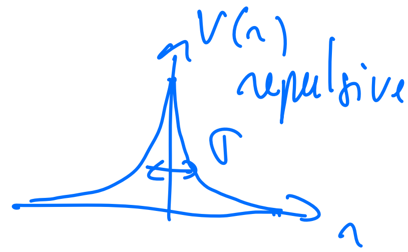
In region (2), Phase-separation is observed.

If $D_t \to 0$, $\left(\frac{v}{\alpha}\right)_c \to 0$; MIPS is seen everywhere.

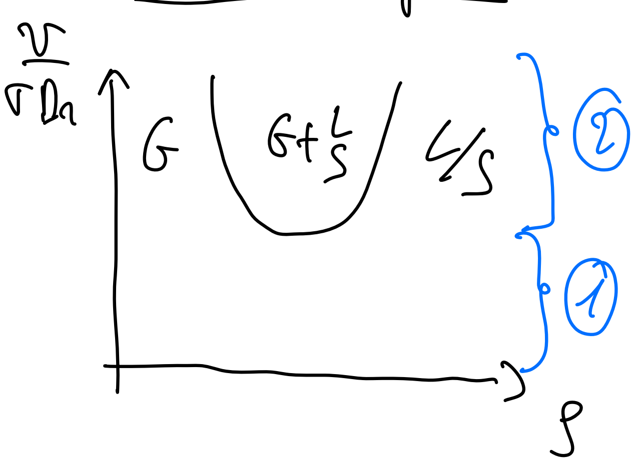
* ABPs: [Fily, Marchetti, PRL 108, 235702 (2012)]
[Redner, Hagan, Baskaran, PRL 110, 055701 (2013)]

→ pairwise forces

$$\begin{cases} \dot{\vec{r}}_i = v_0 \, \vec{u}(\theta_i) - \sum_{j \neq i} \vec{\nabla}_{\vec{r}_i} V(\vec{r}_j - \vec{r}_i) \\ \dot{\theta}_i = \sqrt{2 D_r} \, \xi_i \end{cases}$$



Phase diagram



In region 1, as in equilibrium, pairwise repulsive forces leads to a homogeneous fluid.

In region 2, phase-separation occurs.

END LECTURE 3

* AOUPs: also observed both for pairwise repulsive forces and for quorum sensing interactions.

[Fodor et al, PRL 117, 038103 (2016)]
[Martin et al, arxiv: 2008.12972]