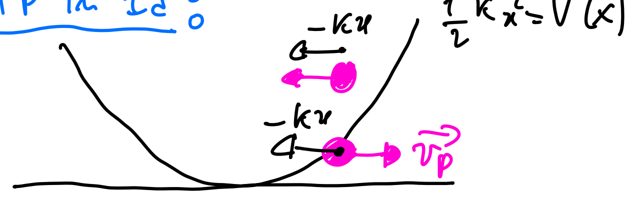
Active particles in external potentials

b) Confinement

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

RTP in 1d:



$v_R = v_p - \kappa x$ $\qquad \alpha_R = \alpha_L = \alpha$

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

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

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

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

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

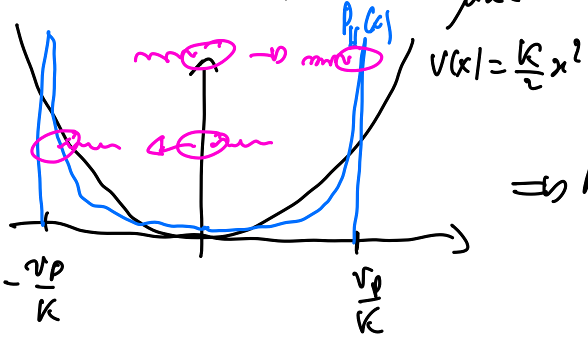
① if $x > \frac{v_p}{\kappa}$ $\quad v_R < 0$; $\quad x < -\frac{v_p}{\kappa}$ $\quad v_L > 0$ $\Big\}$ bounded horizon $\left[-\frac{v_p}{\kappa}, \frac{v_p}{\kappa}\right]$ accessible to the particles

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

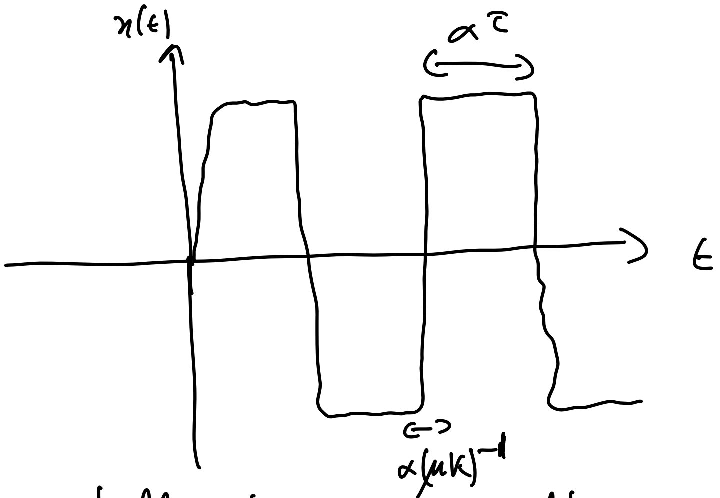
$$\sim e^{-\frac{1}{2\mu\kappa\tau}\cdot\left(\frac{\mu\kappa x}{v_p}\right)^2} = e^{-\frac{\mu\kappa x^2}{2\tau v_p^2}} = e^{-\beta_{eff}\frac{\kappa x^2}{2}}$$

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

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



$\Rightarrow$ Accumulation at the horizon



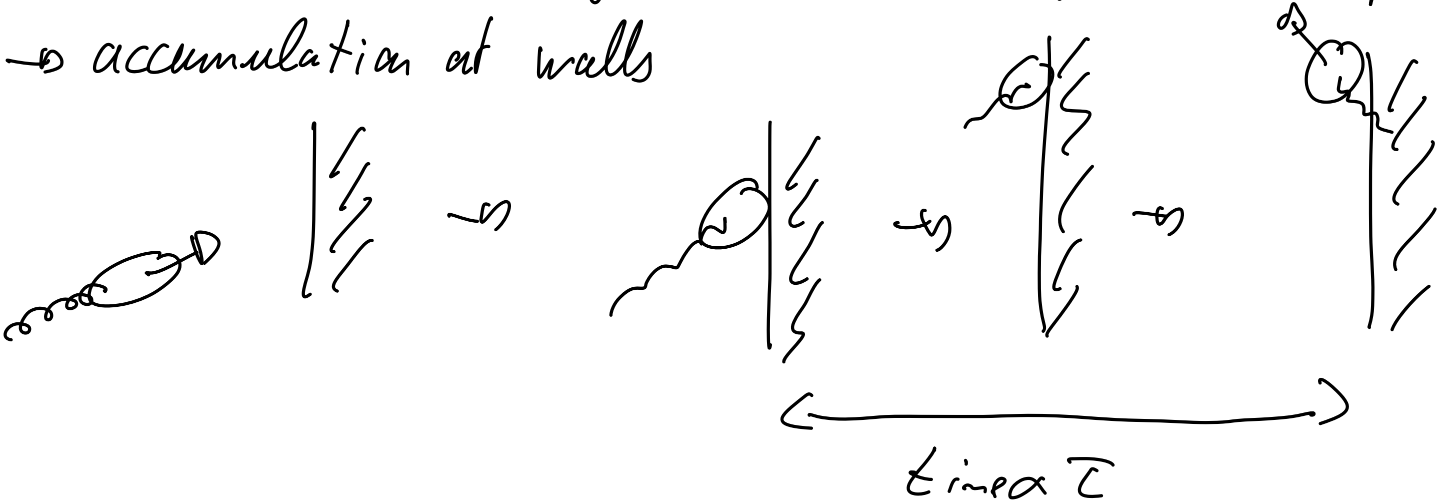
$\Rightarrow$ accumulation at $x = \pm \frac{v_p}{K}$

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

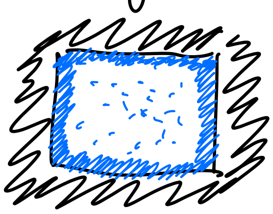
c) active particles and walls

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

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

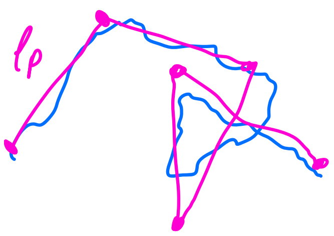
[Elgeti, Gompper, EPL 2009, 2013]

d) the effective equilibrium regime

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.

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

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

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

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

⚠ This works because there are no other sources of fluctuations. If v_0 fluctuates, the relation between ℓ_p, τ & D is not universal.

The equilibrium limit

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.

* This explains the $\tau \to 0$ result for the harmonic well above.

Take home message

① Universal equilibrium regime at $\tau = 0$, D constant

effective temperature : $kT_{eff} = \frac{D}{\mu}$

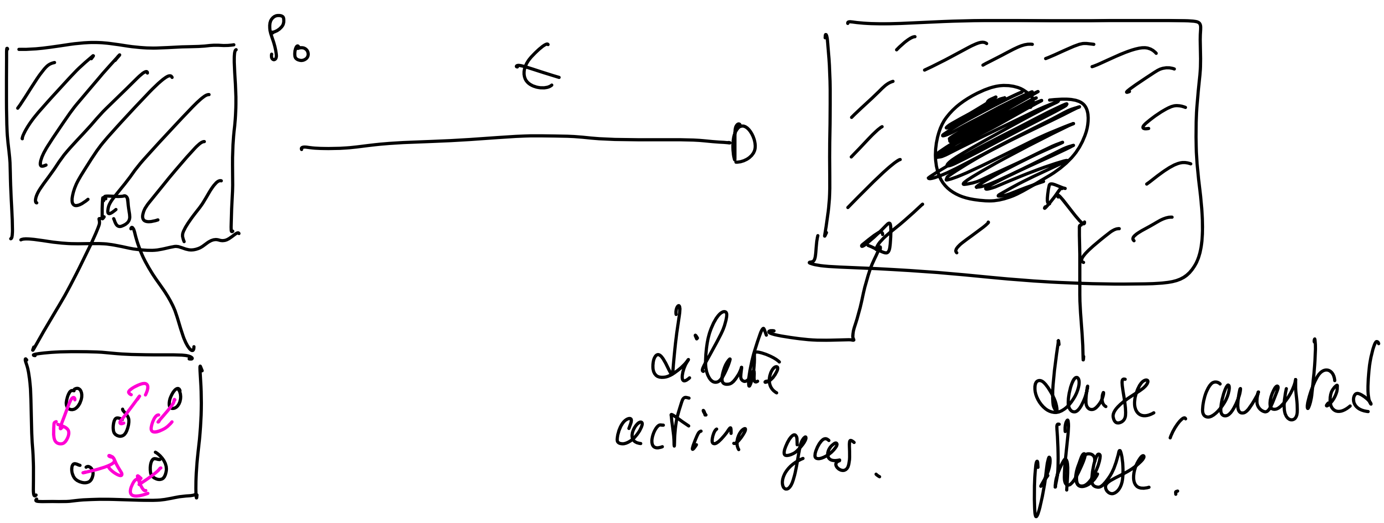
where D is the large scale diffusivity of the particle.

② Large $\tau \Rightarrow$ strong non-equilibrium effects

- accumulation at walls
- gravitational collapse
- non-monotonous $P(x)$ in traps.

7.7) Motility-induced phase separation

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:

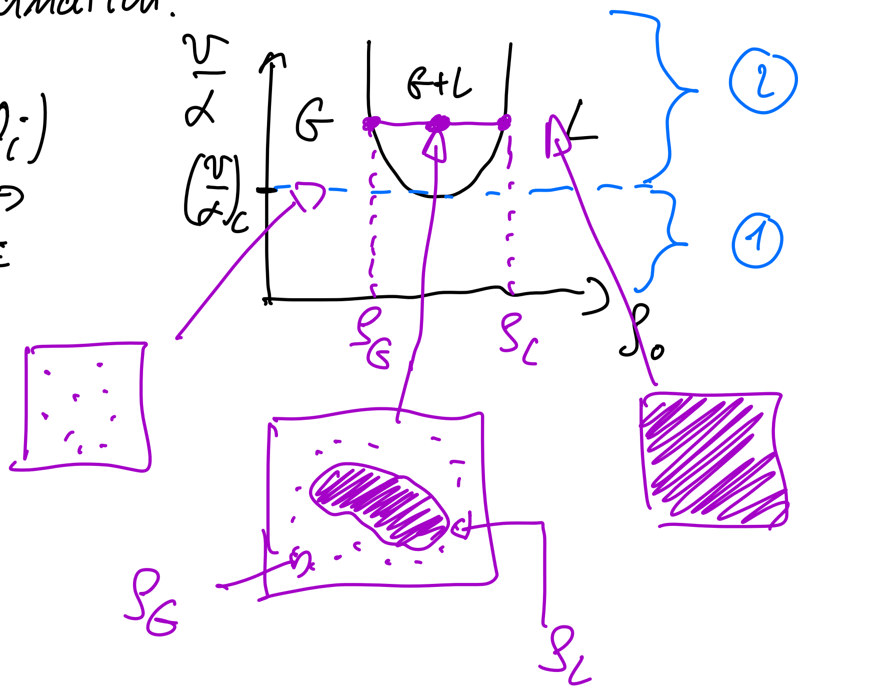
* RTPs [Tailleur, Cates, PRL 101, 218013, (2008)]

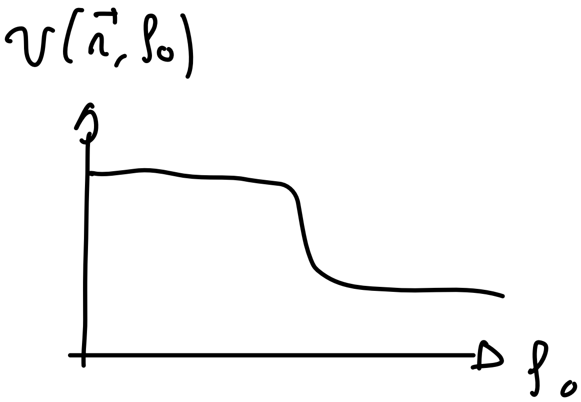
on lattice [Thompson et al., J. Stat. Mech. P 02029, (2011)]

$\Rightarrow$ quorum-sensing information.

$$\dot{\vec{r}}_i = v(\vec{r}_i, [\rho])\,\vec{u}(\theta_i) + \sqrt{2D_t}\,\vec{\eta}_i$$

$$\theta_i \xrightarrow{\alpha} \theta_i'$$





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

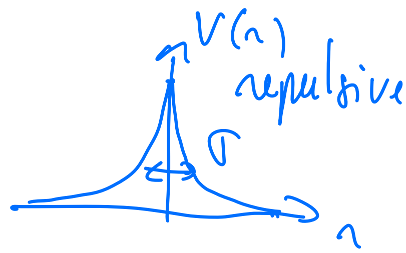
In region (2), Phase-separation is observed.

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

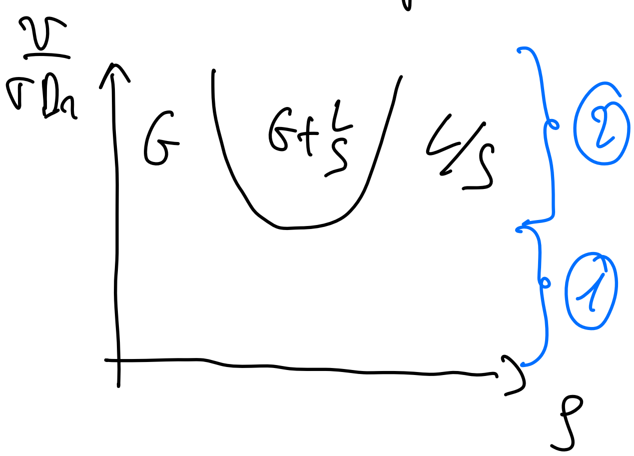
* ABPs : [Fily, Marchetti, PRL 108, 235702 (2012)]
[Redner, Hagan, Baskaran, PRL 110, 055701 (2013)]

→ pairwise forces

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



Phase diagram



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

In region 2, phase-separation occurs.

* In experiments :

→ Enhanced tendency for clustering : [Theurkauff et al, PRL 108, 268303 (2012); Palacci et al., Science 339, 936 (2013)]

→ Phase separation : [Buttinoni et al., PRL 2013, 110, 238301]

→ self-propelled Janus colloids

→ Bacterial colonies : [Liu et al, PRL 122, 248102, (2019)]

→ Quincke rollers: [Geyer et al, PRX 9, 031043 (2019)]
Coexistence between ordered polar active liquid & an arrested solid.

7.7.1) A linear stability analysis

ABP's or RTPs interacting via quorum-sensing interaction $v(\rho(r))$

① Non-uniform speed $v(\vec{r})$ without interactions in 2D with PBC

$$\partial_t P(\vec{r},\theta) = -\vec{\nabla}_{\vec{r}} \cdot [v(r)\,\vec{u}(\theta)\,P(\vec{r},\theta,t)] + \text{isotropic reorientation terms } \Theta \cdot P$$

ABPs: $\Theta P = D_r\, \partial_{\theta\theta} P(\vec{r},\theta)$

RTPs: $\Theta P = -\alpha P(\vec{r},\theta) + \alpha \int \frac{d\theta'}{2\pi} P(\vec{r},\theta')$

Steady-state $\partial_t P(\vec{r},\theta) = 0$

α) $P(\vec{r},\theta) = f(\vec{r})$ then $\Theta P = 0$

β) $\vec{\nabla}_{\vec{r}} \cdot [v(\vec{r})\,\vec{u}(\theta)\,f(\vec{r})] = 0 \Rightarrow f(\vec{r}) = \frac{K}{v(\vec{r})}$

$$\vec{\nabla}_{\vec{r}} \cdot [\underbrace{K\,\vec{u}(\theta)}_{\text{no } \vec{r}\text{-dependency}}] = 0$$

⇒ Steady-state $\boxed{P_{ss}(\vec{r},\theta) = \frac{K}{v(\vec{r})}}$

Active particles spend more time when they go slowly

$\Rightarrow$ accumulation in slow regions

(1) Repulsive force / crowding: model $v(\rho(r))$ with $v'(\rho)<0$

$\Rightarrow$ particles that go slower where are denser.

(1) model a lack of food $\to$ quorum-sensing [Curatolo et al, Nat. Phys. 2020]

(2) pairwise forces

$$\dot{\vec{r}}_i = v_0\,\vec{u}(\theta_i) + \vec{F}_i \;;\quad \vec{F}_i = -\sum_j \vec{\nabla}_{\vec{r}_i} V(\vec{r}_i-\vec{r}_j)$$

$$= \underbrace{\boxed{v_0 + \vec{F}_i\cdot\vec{u}(\theta_i)}\,\vec{u}(\theta_i)}_{} + \left(1-\vec{u}(\theta_i)\,\vec{u}(\theta_i)\right)\vec{F}_i$$

$$= \text{“}v(\rho)\text{”}\;\vec{u}(\theta_i) \;+\; 0$$

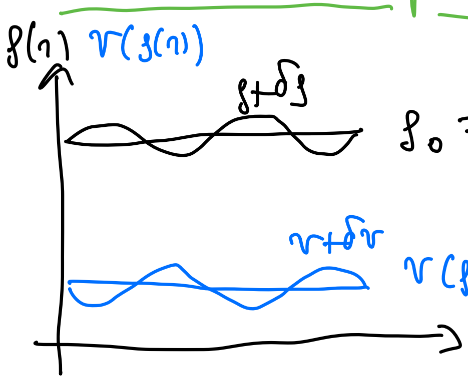
MF + neglect 2nd term.

Repulsive forces lead to a decrease of $v(\rho)$ as

$$v(\rho) \simeq v_0\left(1-\frac{\rho}{\rho^*}\right)$$ [Fily et al, PRL 2012]

crowding density

Feed back loop leading to MIPS:



$$\rho_0 = \frac{K}{v_0}$$

Perturbation $\rho(r) = \rho_0 + \delta\rho(r)$

$$\delta\rho(r) \ll \rho_0$$

Since $v(\rho(r)) = v(\rho_0) + \delta v(r)$

$$= v(\rho_0) + v'(\rho_0)\,\delta\rho$$

Q: where does $\rho(\vec{r})$ wants to relax?

$\rho(\vec{r})$ is a conserved field $\Rightarrow$ its evolution a large scales is <u>slow</u>

Locally particles want to relax towards $\rho(\vec{r}) \propto \frac{k}{v(\vec{r})}$

$$\frac{k}{v(\rho(r))} = \frac{k}{v(\rho_0)+v'(\rho_0)\delta\rho} = \frac{k}{v(\rho_0)} \cdot \frac{1}{1+\frac{v'}{v}\delta\rho} = \underbrace{\frac{k}{v(\rho)}}_{\rho_0}\left(1 - \frac{v'(\rho_0)}{v(\rho_0)}\delta\rho\right)$$

Start from $\rho_0 + \delta\rho$; relax to $\rho_0 - \frac{v'(\rho_0)}{v(\rho_0)}\rho_0\,\delta\rho$

if $|\delta\rho| < \left|-\frac{v'}{v}\rho_0\,\delta\rho\right| \Rightarrow$ perturbation is amplified $\Rightarrow$ instability

linear instability criteria: $\boxed{\frac{v'(\rho_0)}{v(\rho_0)} < -\frac{1}{\rho_0}}$

Conclusion: When $v'(\rho_0)$ is sufficiently negative, this hand-waving argument predicts a linear instability.

Q: Can we derive this quantitatively in a specific model?

Comment: This argument can be made more quantitative and can be generalized to non-vanishing translational diffusion [Cates, Tailleur, Ann. Rev. Cond. Mat. Physics 6, 219-244 (2015)]