Quantum Active Particles from Engineered Dissipation

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YITP
YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Thanks Hisao !

J stat 20th 2004-2024

Editors from the region :

China: Linyuan Lu, Lei-Han Tang, Haijun Zhou

India: Deepak Dhar, Manas Kulkarni, Sriram Ramaswamy, Srikanth Sastry

Japan: Yoshiyuki Kabashima, Shin-ichi Sasa

Korea: Doochul Kim, Jae Sung Lee

Plan

1. Classical Active Matter
   - Real and artificial systems
   - Models
   - Phenomenology
2. Quantum Active Matter
   - Models
   - Phenomenology
   - Realizations ?
3. Perspectives

Plan

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Active Matter

Definition - Biological inspiration

Active matter is composed of large numbers of active "agents", which consume energy and thus move or exert mechanical forces

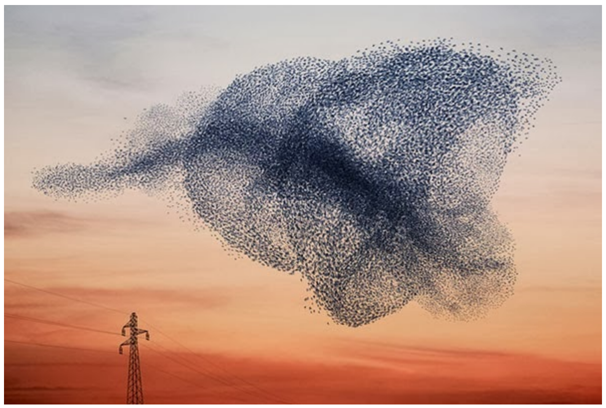
Due to the energy consumption, these systems are intrinsically out of thermal equilibrium

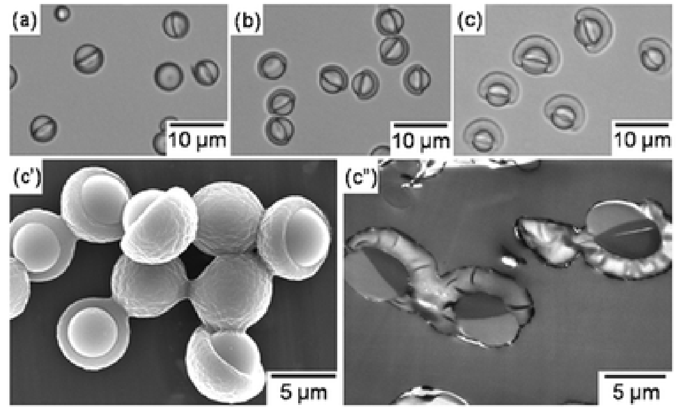
Homogeneous energy injection (not from the borders, *cfr.* shear)

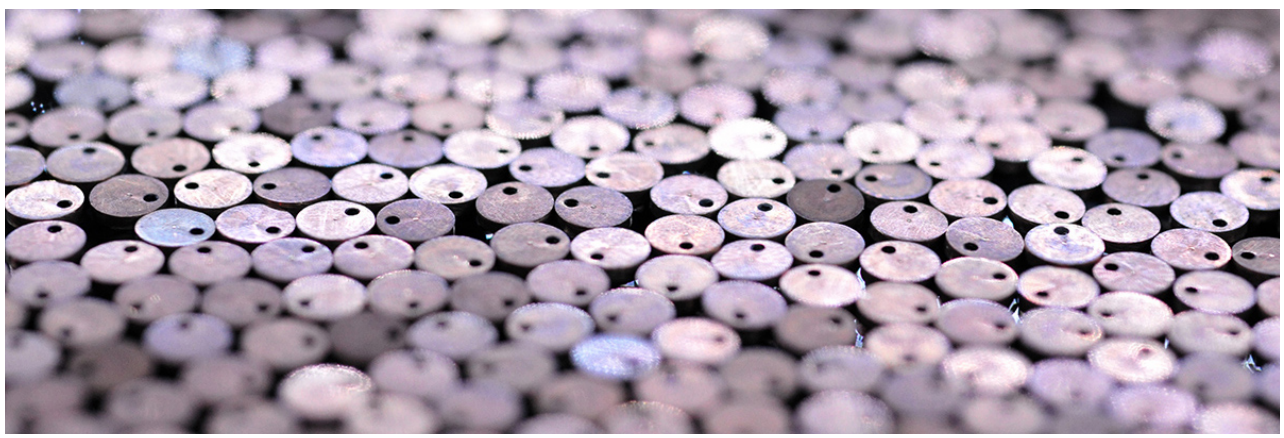
Coupling to the environment (bath) allows for dissipation

Active Matter

Natural & artificial systems







Experiments & observations **Bartolo et al.** Lyon, **Bocquet et al.** Paris, **Cavagna et al.** Roma, **di Leonardo et al.** Roma, **Dauchot et al.** Paris, just to mention some Europeans

Active Matter

Global goal - from our "community"

To understand the **collective** behaviour of **active matter**

from the **statistical physics** viewpoint

with the help of extensive **numerical simulations**

and **theoretical arguments/analytic calculations**

Statistical Physics approach

But, one has to start from the **single particle** modeling

Brownian Motion

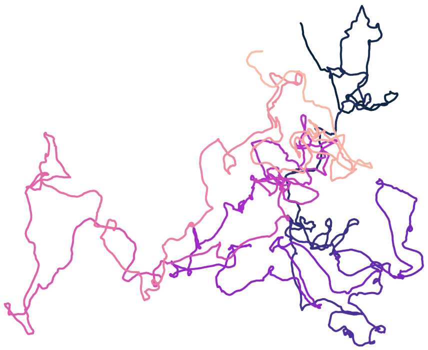
Langevin description

A spherical particle immersed in a liquid

Force on the particle due to the coupling to the environment

No external force

$$\overbrace{m\ddot{\mathbf{r}} \;=\; \mathbf{F}_{\text{env}}}^{\text{Newton}} \;=\; \underbrace{-\,\gamma\dot{\mathbf{r}}}_{\text{friction}} + \underbrace{\boldsymbol{\xi}}_{\text{noise}}$$



$\boldsymbol{\xi}$ Gaussian white noise with $\langle \xi_a(t) \rangle = 0$ and $\langle \xi_a(t)\xi_b(t') \rangle = 2\gamma k_B T \delta_{ab}\delta(t-t')$

$a, b = 1, \ldots, d$

Averaged position $\langle \mathbf{r}(t) \rangle = \mathbf{r}_0$ the initial position

Brownian Motion

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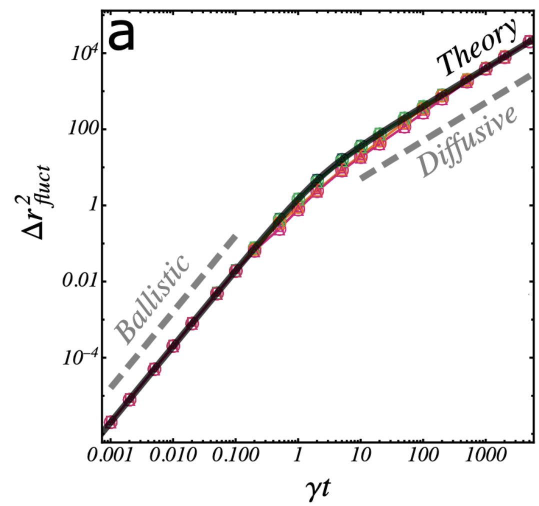


Mean-square displacement

$$\Delta^2(t,0) = \langle(\mathbf{r}(t) - \mathbf{r}_0)^2\rangle$$

At $t < {}^{m}/_{\gamma}$ *ballistic* $\Delta^2 \propto t^2$

At $t > {}^{m}/_{\gamma}$ *diffusive* $\Delta^2 \propto D_T\, t$

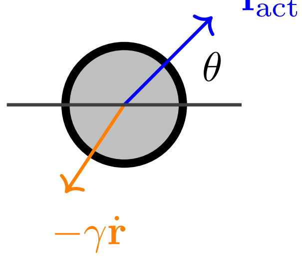
Diffusion coefficient $D_T = {}^{k_B T}/_{\gamma}$

Active Brownian Particle

Langevin equations

Active force $f_{\rm act}$ along $\hat{\mathbf{n}} = (\cos\theta, \sin\theta)$ a direction following a random walk

$$
\begin{aligned}
m\ddot{\mathbf{r}} &= f_{\rm act}\hat{\mathbf{n}} - \gamma\dot{\mathbf{r}} + \boldsymbol{\xi} \\
\dot{\theta} &= \eta
\end{aligned}
$$



$\boldsymbol{\xi}$ and η Gaussian white noises

$\langle \xi_a(t)\rangle = \langle \eta(t)\rangle = 0$, $\langle \xi_a(t)\,\xi_b(t')\rangle = 2\gamma k_B T \delta_{ab}\delta(t-t')$ and $\langle \eta(t)\,\eta(t')\rangle = 2D_\theta\delta(t-t')$

Persistence time $\tau_p = 1/D_\theta$ and length $\ell_p = v_0\,\tau_p = (f_{\rm act}/\gamma)\,\tau_p$

Péclet number Pe = $f_{\rm act}\sigma/(k_B T)$ measures the activity

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Active Ornstein Uhlenbeck Process

Over-damped Langevin equations

Long times, beyond the inertia time-scale $t \gg {}^{m}\!/\!_{\gamma}$

$$\dot{\mathbf{r}} = \mathbf{v} \qquad\qquad \tau\,\dot{\mathbf{v}} = -\mathbf{v} + \eta$$

Gaussian white noise with $\langle \eta_a(t) \rangle = 0$ and $\langle \eta_a(t)\eta_b(t') \rangle = 2D\,\delta_{ab}\,\delta(t-t')$

The random velocity $\mathbf{v}$ is correlated as

$$\langle v_a(t) v_b(t') \rangle = \delta_{ab}\,\frac{D}{\tau}\,e^{-|t-t'|/\tau}$$

Unbalanced correlated noise and memoryless friction $\Longrightarrow$

out-of-equilibrium environment

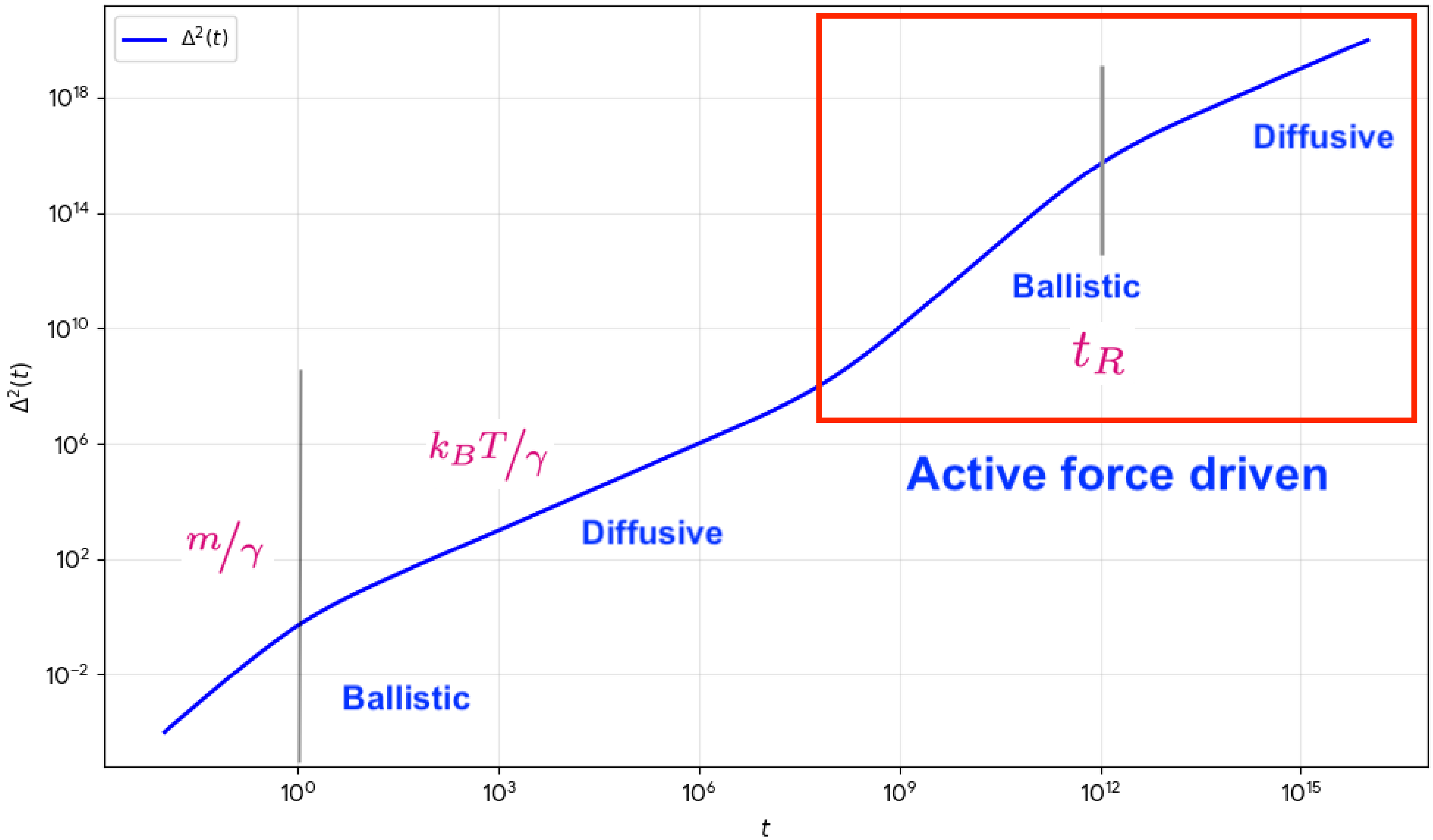
Similar **phenomenology** as the one of the ABPs but simpler to deal with,

no additional degree of freedom **Martin et al 2021**

ABP & AOUP

Mean-square displacement

$$\Delta^2(t) \equiv \langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \rangle = \langle (\mathbf{r}(t) - \mathbf{r}_0)^2 \rangle = \langle (\mathbf{r}(t) - \langle \mathbf{r}(t) \rangle)^2 \rangle \equiv \mathrm{Var}(\mathbf{r}(t))$$



Active Brownian Particle

Mean-square displacement

Active force $f_{\rm act}$ along $\hat{\mathbf{n}} = (\cos\theta, \sin\theta)$ a direction following a random walk

$$m\ddot{\mathbf{r}} = f_{\rm act}\hat{\mathbf{n}} - \gamma\dot{\mathbf{r}} + \boldsymbol{\xi} \qquad\qquad \dot{\theta} = \eta$$

Mean-square displacement $\quad \Delta^2(t) = \langle(\mathbf{r}(t) - \mathbf{r}(0))^2\rangle$

Time	Regime	$\Delta^2 \propto$	Physical Interpretation
$t < {}^{m}/_{\gamma}$	ballistic	${}^{k_B T}/_{m}\; t^2$	Inertial thermal velocity dominates
${}^{m}/_{\gamma} < t < \tau^*$	diffusive	$D_T\; t$	Damping $\mapsto$ thermal Brownian motion
$\tau^* < t < t_R$	ballistic	${}^{f_{\rm act}^2}/_{\gamma^2}\; t^2$	Self-prop speed $v_0 = {}^{f_{\rm act}}/_{\gamma}$ dominates
$t_R < t$	diffusive	$D_A\; t$	Rotational diff randomizes $\mathbf{v}_0$

Diffusion coefficients $\quad \underbrace{D_T = {}^{k_B T}/_{\gamma}}_{\text{thermal}} \qquad \underbrace{D_A = D_T + c\,\mathrm{Pe}^2}_{\text{active}}$

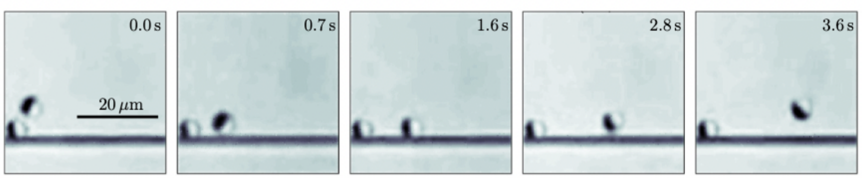
Active Brownian Particle

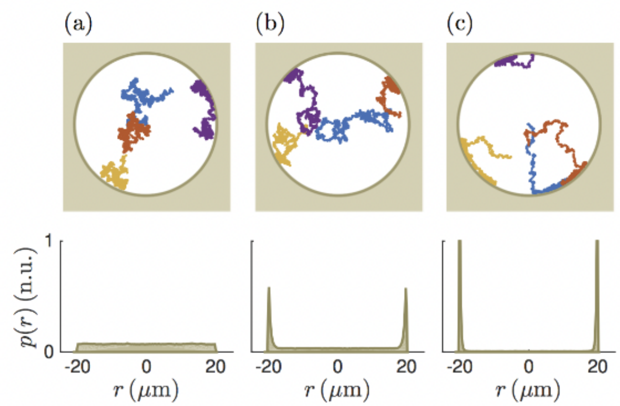
Aggregation close to walls

Active force f_{act} along $\hat{\mathbf{n}} = (\cos\theta, \sin\theta)$ a direction following a random walk

$$m\ddot{\mathbf{r}} = f_{\mathrm{act}}\hat{\mathbf{n}} - \gamma\dot{\mathbf{r}} + \boldsymbol{\xi} \qquad \dot{\theta} = \eta$$

Motion of Janus colloids & ABPs

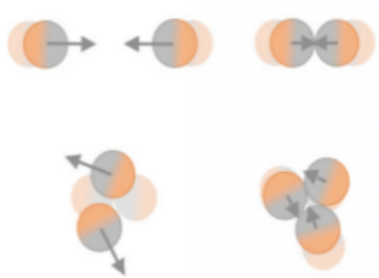




close to a wall **in a pore**

Motility Induced Phase Separation

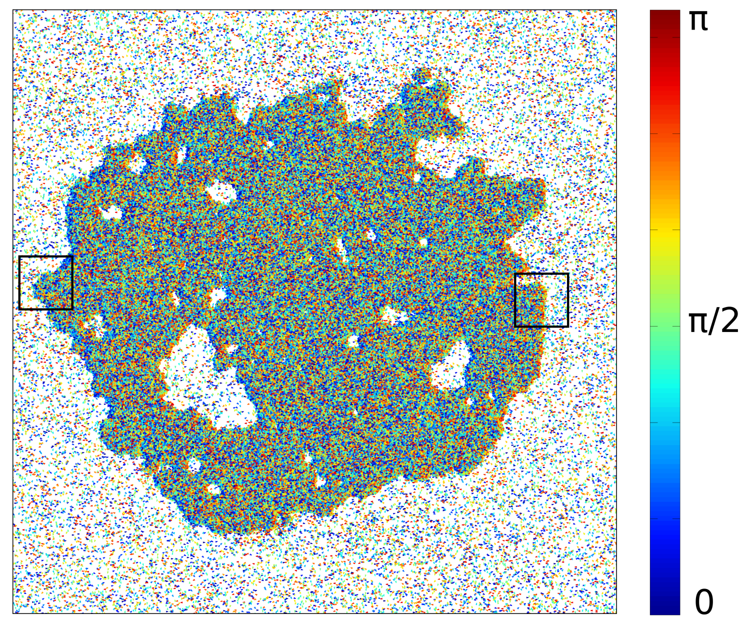
The basic mechanism



Particles collide heads-on

and cluster even in the

absence of attractive forces



$\longrightarrow$ **blue 0** $\longleftarrow$ **red** π

The colours indicate the direction $\mathbf{n}_i$ along which the particles are pushed by the active force $f_{\rm act}$

Tailleur & Cates 08

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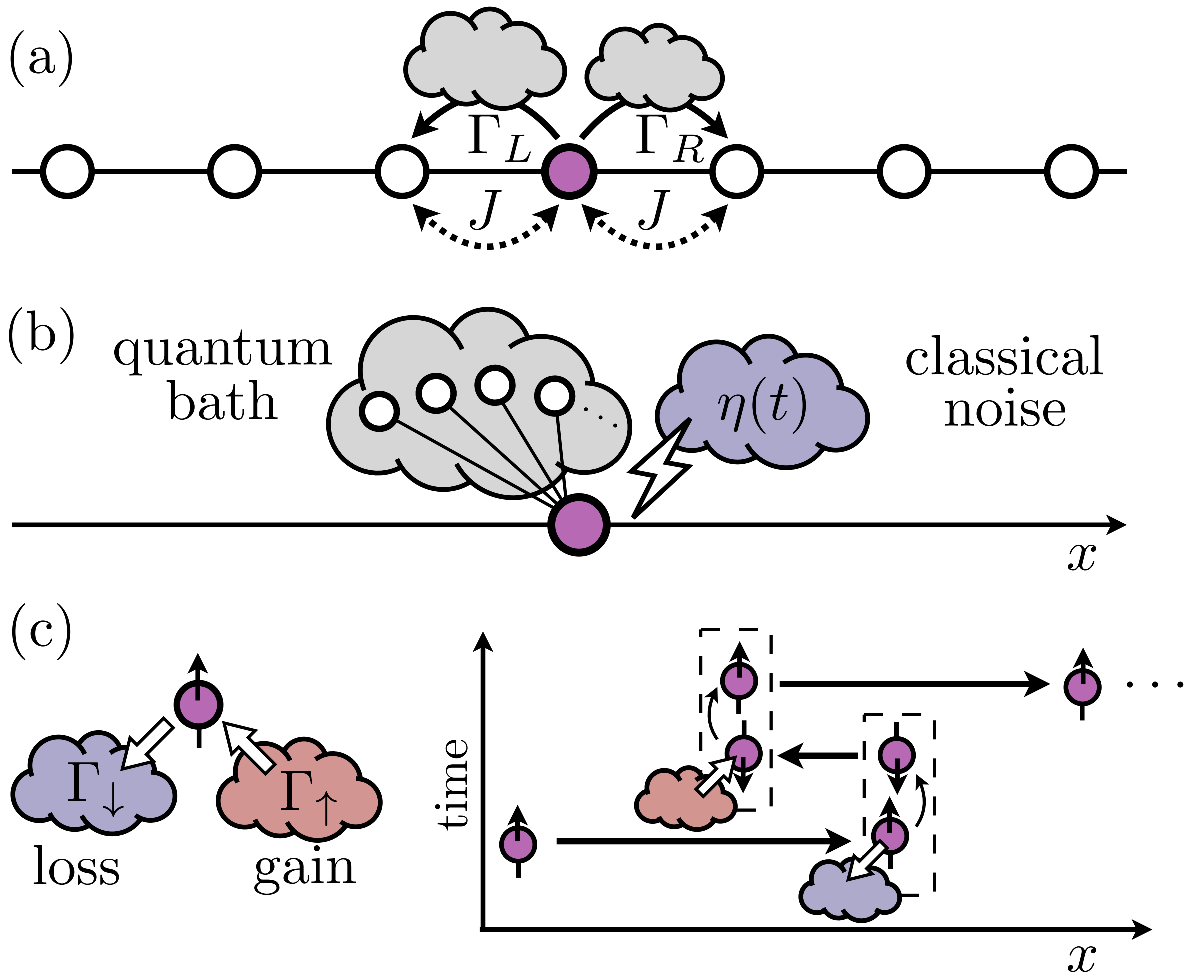
Quantum Active Particles

Sketches of three models - playing with the environments



Quantum Active Particles

Purely quantum models (a) and (c)

Take a system with a time-independent Hamiltonian $\hat{\mathcal{H}}$

in a generic mixed state described by the density operator $\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$

with, e.g. $\{|\psi_\alpha\rangle\}$ a basis of Hilbert space & $\sum_\alpha p_\alpha = 1$

and in contact with an environment

The density operator ($\{p_\alpha\}$) depends on time and $\hat{\rho}$ obeys the **Lindblad eq**

$$\underbrace{\partial_t \hat{\rho} = -\frac{\mathrm{i}}{\hbar}\,[\hat{\mathcal{H}}, \hat{\rho}]}_{\text{Heisenberg}} + \underbrace{\sum_n \left(\hat{L}_n \hat{\rho} \hat{L}_n^\dagger - \frac{1}{2}\,\{\hat{L}_n^\dagger \hat{L}_n, \hat{\rho}\} \right)}_{\text{effect of the bath}}$$

where $\{\hat{L}_n\}$ are operators describing the effect of the environment

NB this eq is local in time - **no memory**

Choose $\hat{\mathcal{H}}$ and $\{\hat{L}_n\}$

Quantum Active Particles

Purely quantum models (a) and (c)

Take a system with a time-independent Hamiltonian $\hat{\mathcal{H}}$

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with, e.g., $\{|\psi_\alpha\rangle\}$ a basis of the Hilbert space & $\sum_\alpha p_\alpha = 1$

and in contact with an environment

The observables are calculated as, e.g.,

$$\mathrm{Var}(\hat{x}(t)) = \langle(\hat{x}(t) - \langle\hat{x}(t)\rangle)^2\rangle$$

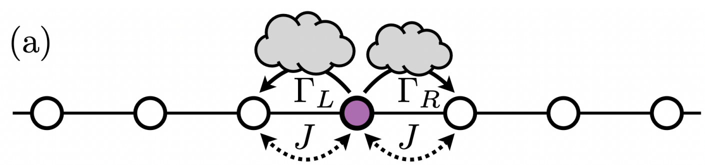
with $\langle\hat{A}(t)\rangle = \mathrm{Tr}(\hat{A}\hat{\rho}(t))$

a bit like the Fokker-Planck description of the classical problems (no memory)

Choose $\hat{\mathcal{H}}$ and $\{\hat{L}_n\}$

Environment-assisted hopping

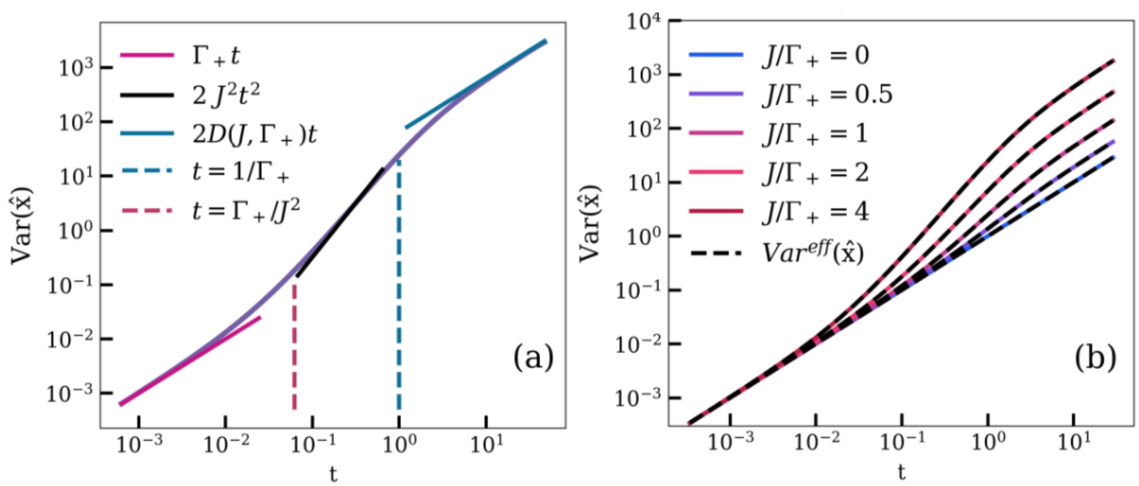
on a one dimensional lattice with periodic boundary conditions



$$\hat{\mathcal{H}} = J \sum_{i=1} \left(\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i \right)$$

where i labels the lattice sites and J is the coherent symmetric hopping rate

Dissipative hopping with $\hat{L}_{i,L} = \sqrt{\Gamma_L}\, \hat{c}_i^\dagger \hat{c}_{i+1}$ and $\hat{L}_{i,R} = \sqrt{\Gamma_R}\, \hat{c}_{i+1}^\dagger \hat{c}_i$



Diffusive Ballistic Diffusive $D = \frac{\Gamma_+}{2}\left(1 + \frac{4J^2}{\Gamma_+^2}\right)$

$$2\Gamma_+ = \Gamma_L + \Gamma_R$$

Crossover times

$$\tau^* = \Gamma_+/J^2$$

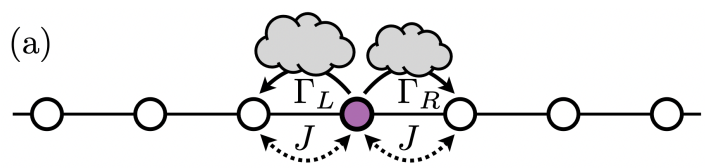
$$t_R = 1/\Gamma_+$$

Effective Péclet

$$\mathrm{Pe} = J/\Gamma_+$$

Environment-assisted hopping

on an open one dimensional lattice with length L



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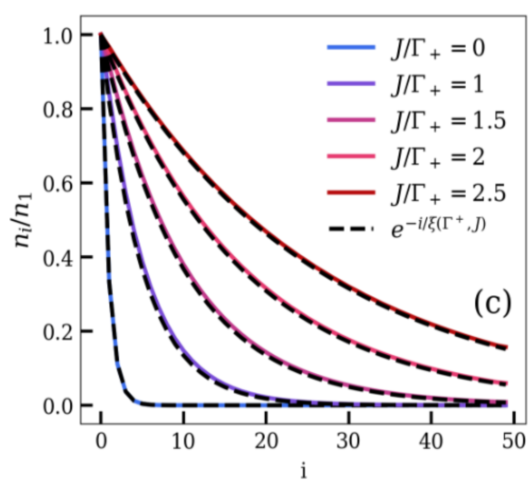


Asymptotic density profile

$$\Gamma_- = \Gamma_L - \Gamma_R > 0$$

$$n_i/n_1 = e^{-(i-1)/\xi}$$

$$\xi \sim \frac{D}{\Gamma_-} = \frac{\text{Diffusion}}{\text{Drift}}$$

as in **Tailleur & Cates 08, Razin 20**

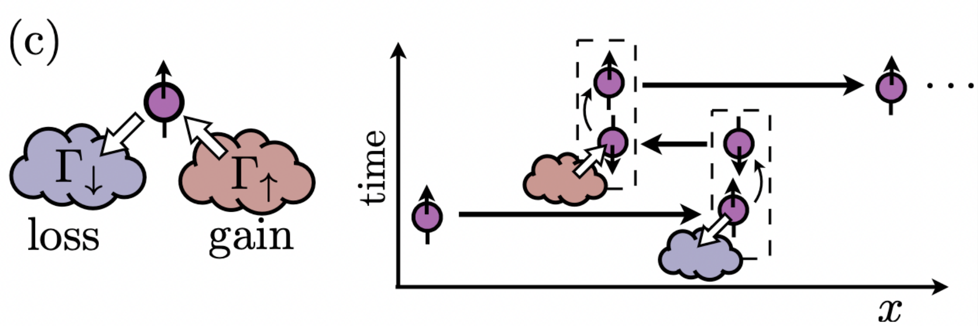
for classical active particles

Lindblad skin effect

Quantum ABP

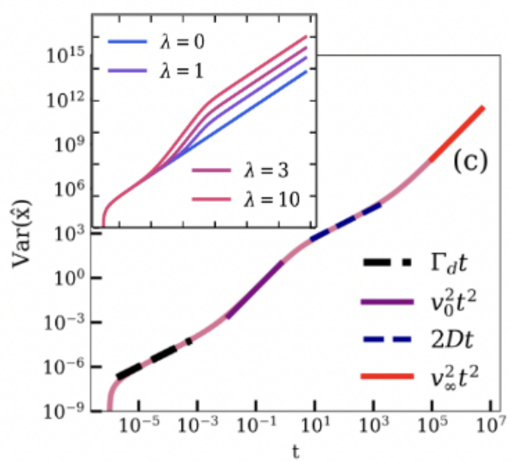
Additional - internal - two-level variable

The internal spin flips couple to left-right motion on the continuous line



$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \lambda\,\hat{p}\hat{\sigma}_z$$

with $\hat{L}_\uparrow = \sqrt{\Gamma_\uparrow}\,\hat{\sigma}_+$ $\hat{L}_\downarrow = \sqrt{\Gamma_\downarrow}\,\hat{\sigma}_-$ $\hat{L}_d = \sqrt{\Gamma_d}\,\hat{p}$



$$2\hat{\sigma}_\pm = \hat{\sigma}_x \pm \mathrm{i}\hat{\sigma}_y$$

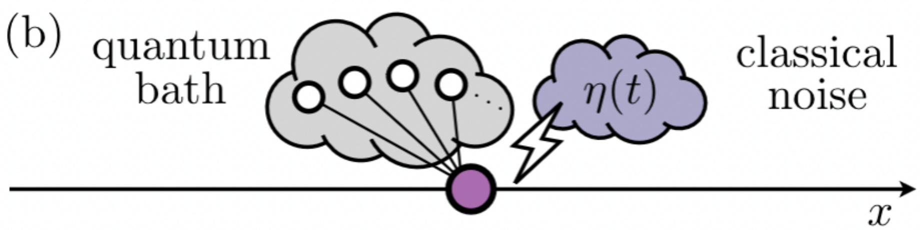
Translation & internal d.o.f. feel different baths

$$D = \frac{\Gamma_d}{2}\left(1 + \frac{2\lambda^2}{\Gamma_d(\Gamma_\uparrow + \Gamma_\downarrow)}\right)$$

last ballistic regime

Quantum Active Particles

similar to Ornstein-Uhlenbeck



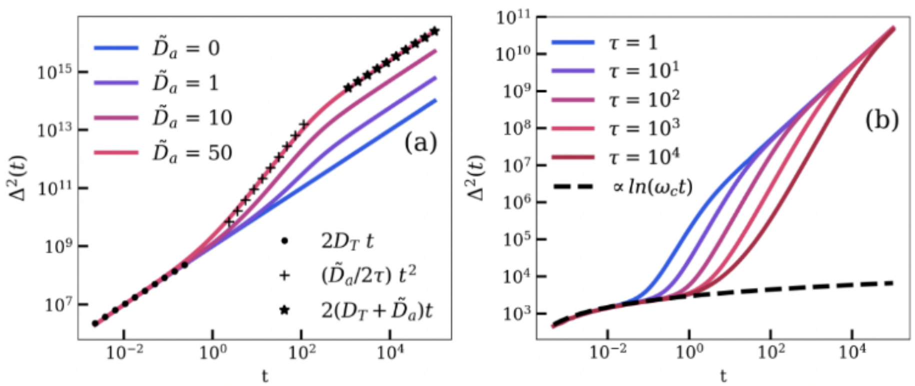
Ohmic quantum dissipation

$$\hat{\mathcal{H}}_{\text{bath}}(\hat{x}) = \sum_\alpha \left(\frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} \hat{x}_\alpha^2 \right) + \hat{x} \sum_\alpha g_\alpha \hat{x}_\alpha$$

$$\hat{\mathcal{H}}_{\text{qAOUP}} = \frac{\hat{p}^2}{2m} + \hat{\mathcal{H}}_{\text{bath}}(\hat{x}) + g \hat{x} \eta(t)$$

spectrum $J(\omega) = \sum_\alpha \frac{g_\alpha^2}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha)$
$= 4\gamma\omega \exp(-\omega/\omega_c)$

The classical noise $\eta(t)$ has zero mean and $\langle \eta(t)\eta(t') \rangle = \frac{D_\eta}{\tau} e^{-|t-t'|/\tau}$



Schwinger-Keldysh - Closed time path integral

Diffusive – Ballistic – Diffusive

$$\tilde{D}_a = D_\eta / 4\gamma^2$$

$$D = D_T + \tilde{D}_a$$

Quantum Active Particles

Realizations

(a) **Environment assisted hopping on a lattice**

- Laser assisted hopping

(b) **Quantum Ornstein - Uhlenbeck particles**

- Superconducting circuits & Josephson junctions
- Impurities in cold atoms
- Optomechanics

(quantum Brownian motion) supplemented by a colored

non-Markovian classical noise

(c) **Quantum Active Brownian Particles**

- Spin-to-momentum coupling can be engineered in atomic physics

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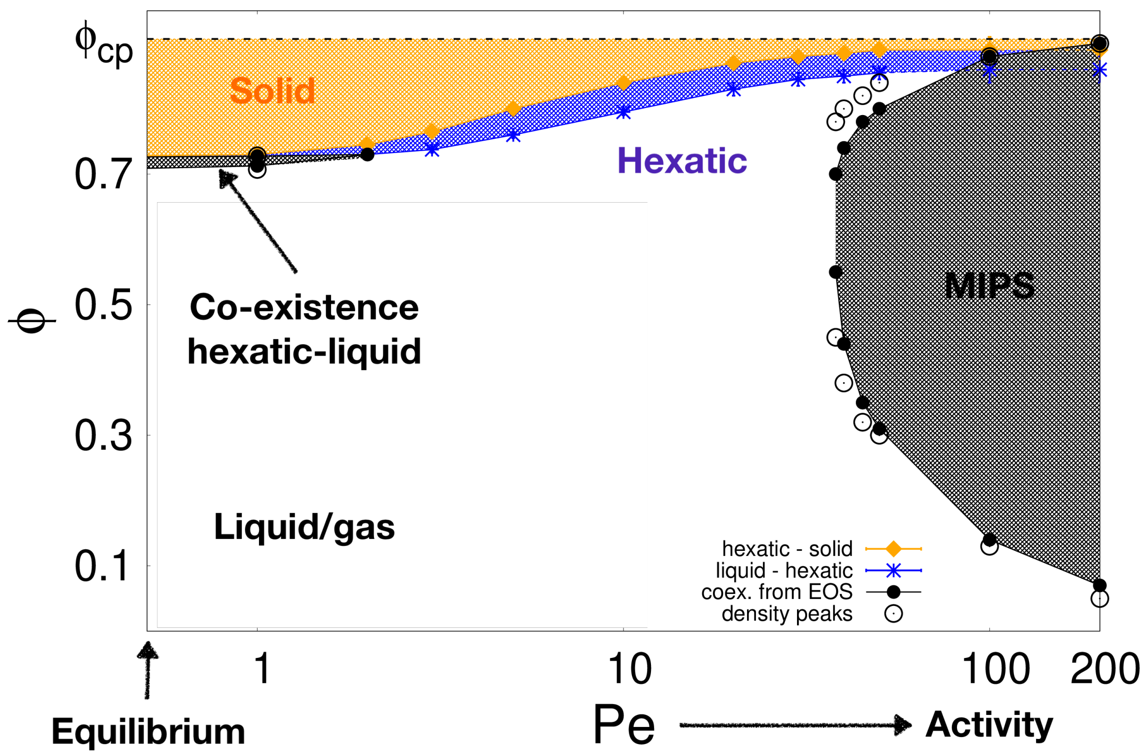
Perspectives

Collective behaviour



Gray zone at high Pe

Motility induced

phase separation (MIPS)

gas & dense

Cates & Tailleur

Ann. Rev. Cond. Matt. 6, 219 (2015)

Farage, Krinninger & Brader

PRE 91, 042310 (2015)

Pressure $P(\phi, \text{Pe})$ (EOS), correlations $G_T(r)$, $G_6(r)$, and distributions of ϕ_i, $|\psi_{6i}|$

Digregorio, Levis, Suma, LFC, Gonnella & Pagonabarraga, PRL 121, 098003 (2018)