Quantum Active Particles from Engineered Dissipation

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Plan

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

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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

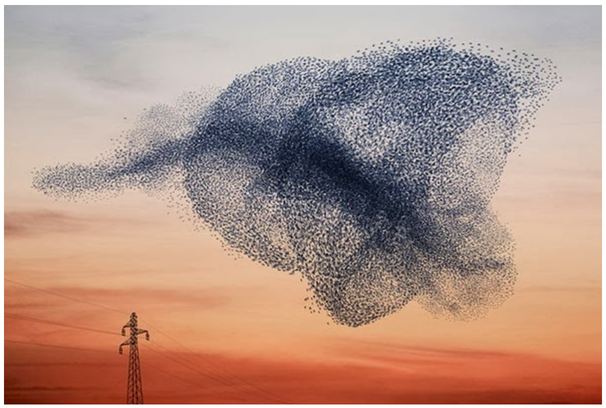
Due to the energy consumption, these systems are intrinsically out of thermal equilibrium

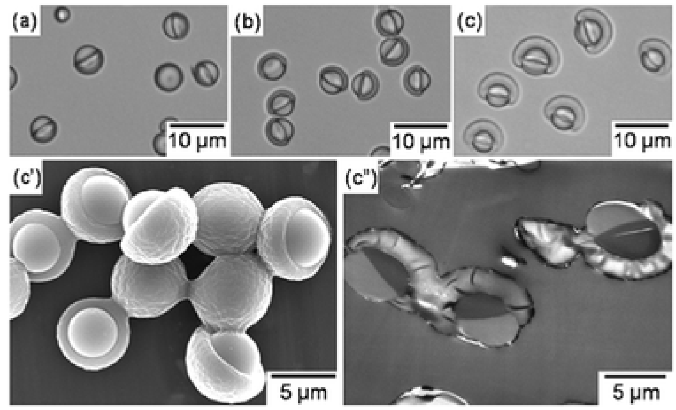
Homogeneous energy injection (not from the borders, *cfr.* shear)

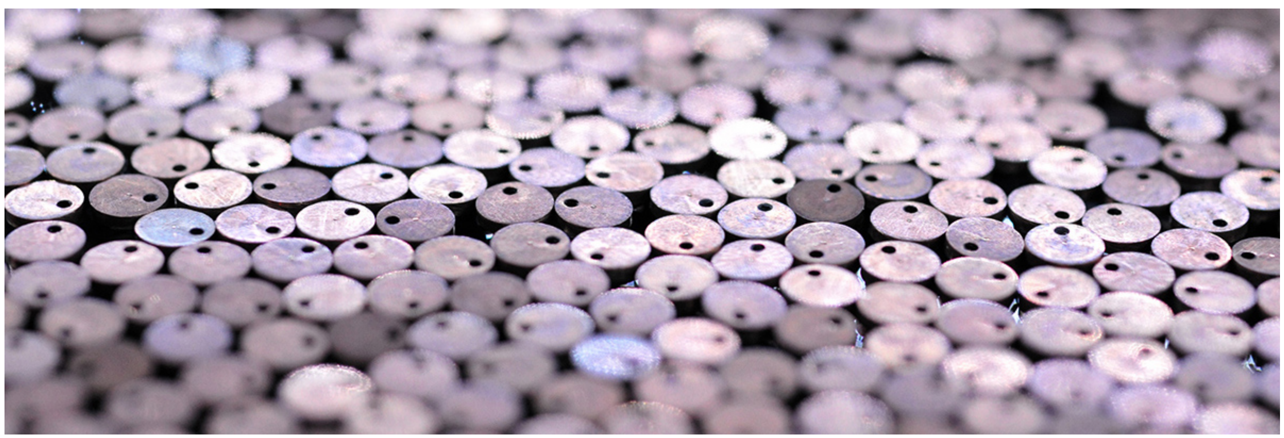
Coupling to the environment (bath) allows for dissipation

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

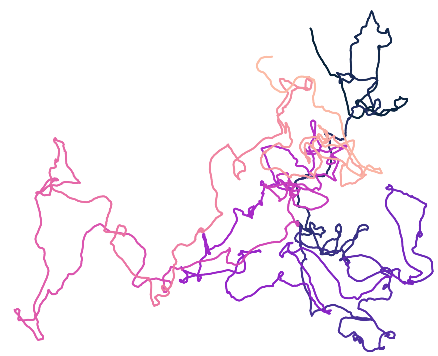
Langevin description

A spherical particle immersed in a liquid

Force on the particle due to the coupling to the environment

No external force

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



$\boldsymbol{\xi}$ 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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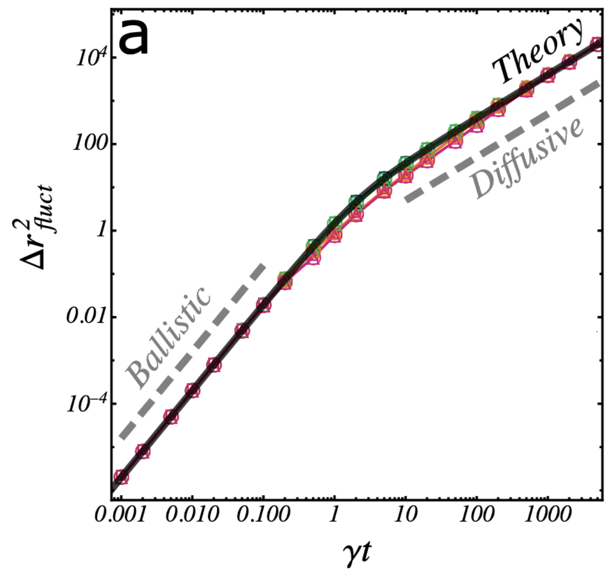


Mean-square displacement $\quad \Delta^2(t,0) = \langle (\mathbf{r}(t) - \mathbf{r}_0)^2 \rangle$

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

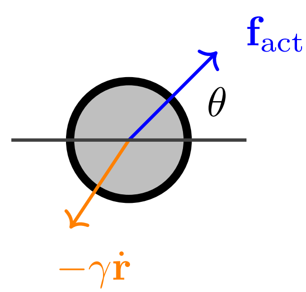
At $t > {}^m\!/\!{}_\gamma$ diffusive $\Delta^2 \propto t$

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

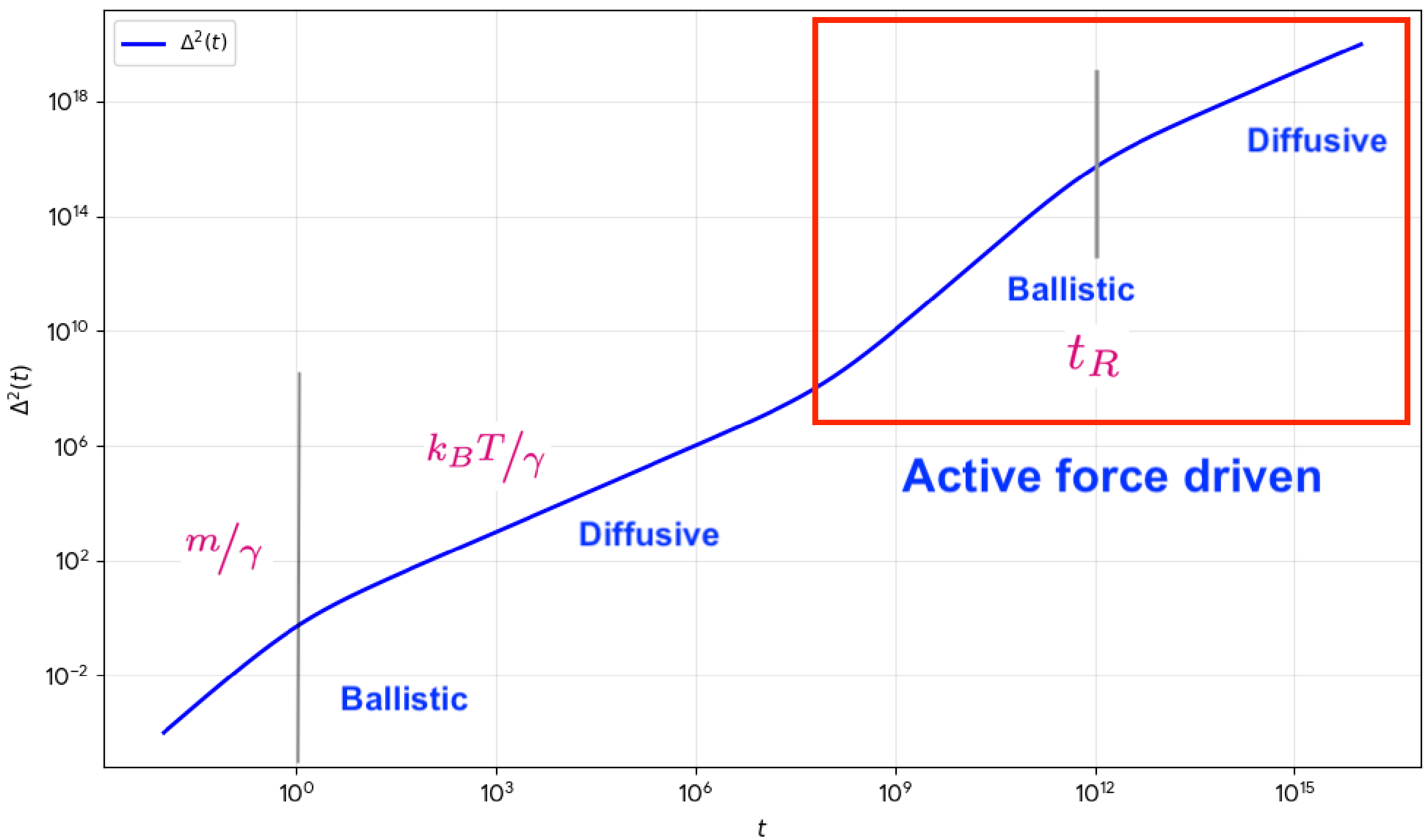
Similar **phenomenology** as the one of the ABPs but simpler to deal with,

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

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

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	$f_{\text{act}}^2/\gamma^2\ t^2$	Self-prop speed $v_0 = f_{\text{act}}/\gamma$ dominates
$t_R < t$	diffusive	$D_A\ t$	Rotational diff randomizes $\mathbf{v}_0$

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

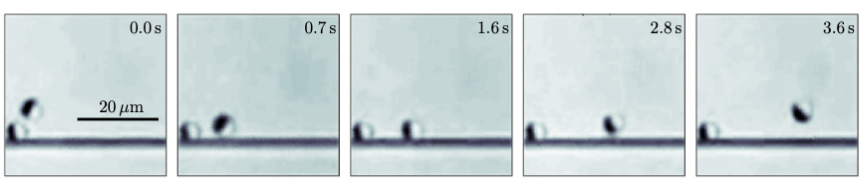
Active Brownian Particle

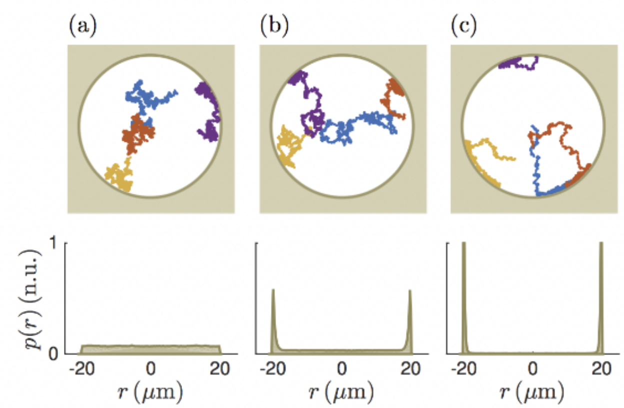
Aggregation close to walls

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

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

Motion of Janus colloids & ABPs





close to a wall | **in a pore**

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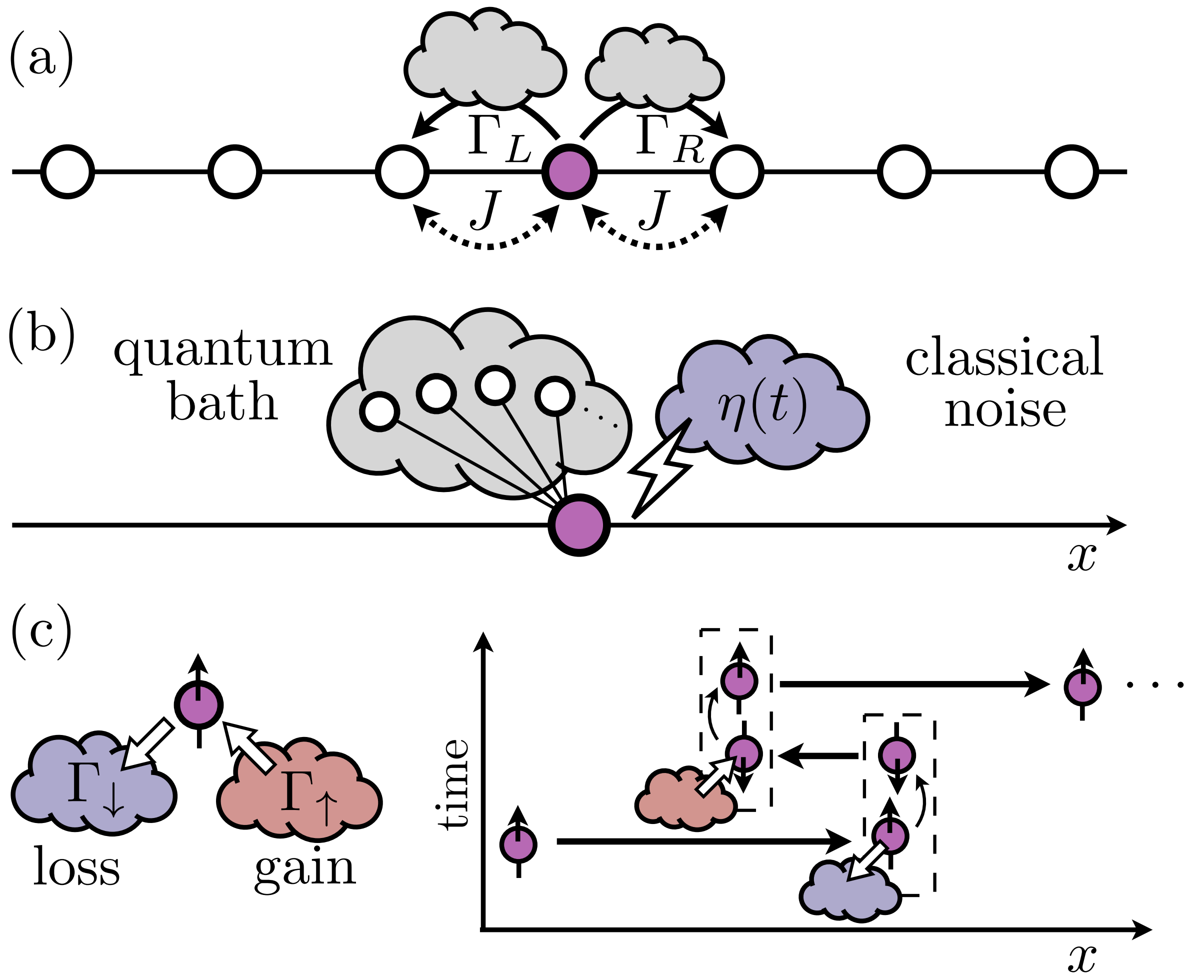
Quantum Active Particles

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 $\{|\psi_\alpha\rangle\}$ a basis of Hilbert space

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 $\hat{\mathcal{H}}$

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 the Hilbert space

and in contact with an environment

The observables are calculated as, e.g.,

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

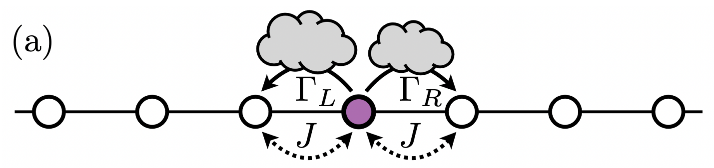
with $\langle\hat{A}(t)\rangle = \mathrm{Tr}(\hat{A}\hat{\rho}(t))$

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

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

Environment-assisted hopping

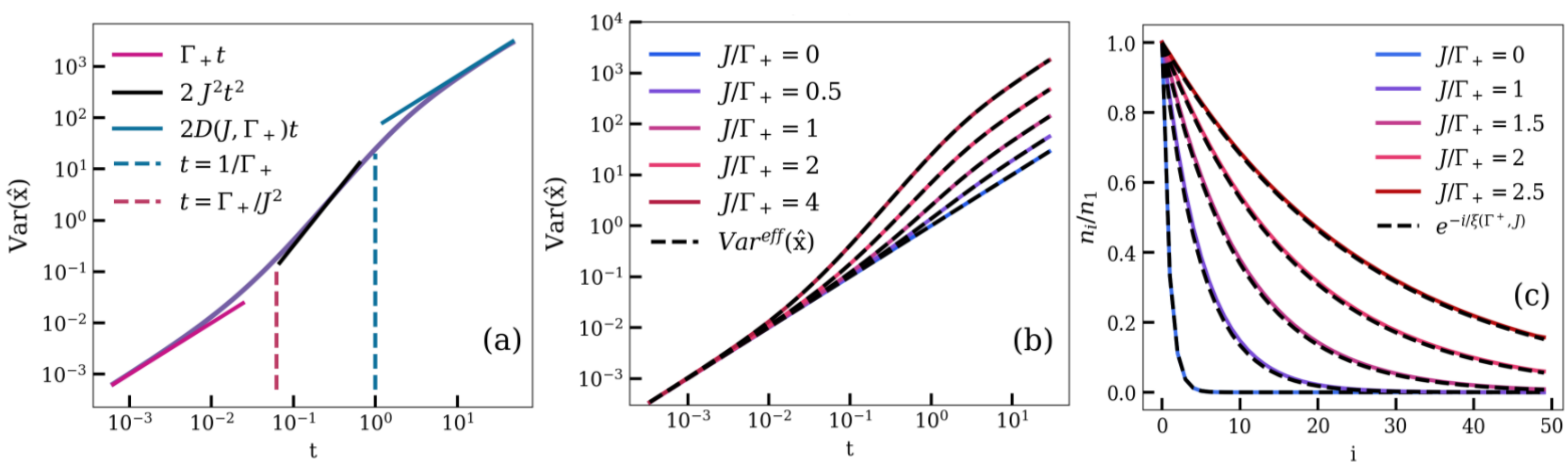
on a one dimensional lattice



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

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

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

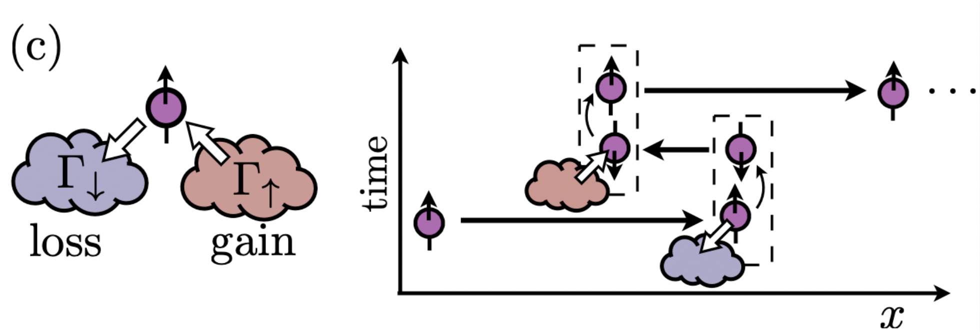


Diffusive Ballistic Diffusive $D = \frac{\Gamma_+}{2}\left(1 + \frac{4J^2}{\Gamma_+^2}\right)$ Density profile

Quantum ABP

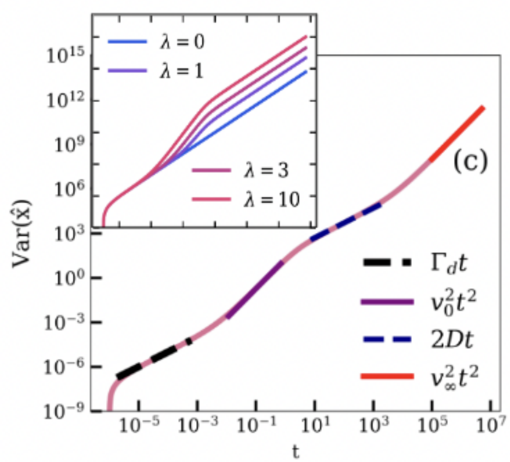
Additional - internal - two-level variable

A particle with an internal spin moving on a continuous line



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

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



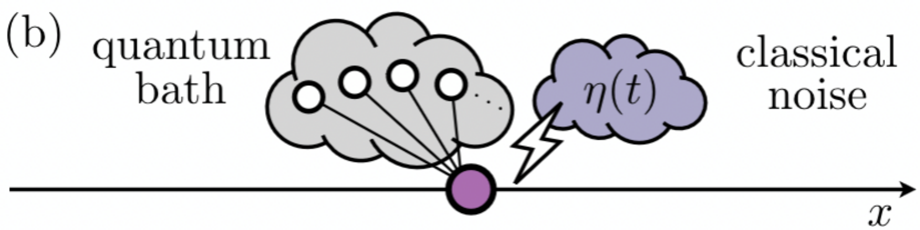
Translation & internal d.o.f. feel different baths

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

last ballistic regime

Quantum Active Particles

similar to Ornstein-Uhlenbeck



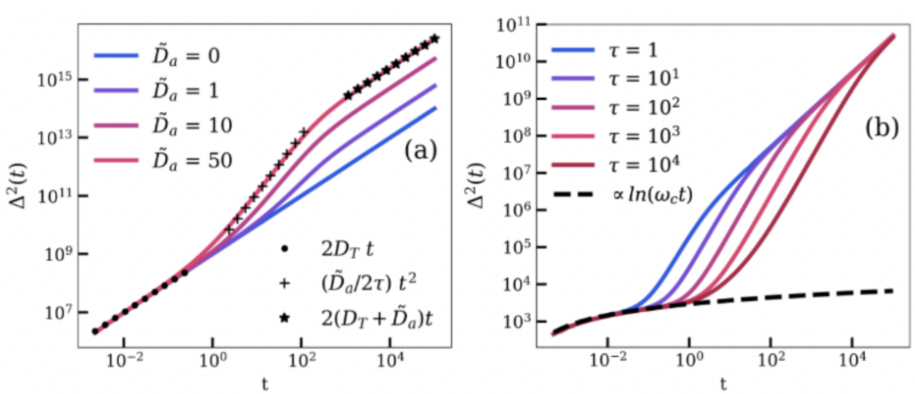
Ohmic quantum dissipation

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

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

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 $\langle \eta(t)\eta(t')\rangle = \frac{D_\eta}{\tau} e^{-|t-t'|/\tau}$



Diffusive Ballistic Diffusive

$$D_a = D_\eta / 4\gamma^2$$

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

Quantum Active Particles

Realizations

1. Model (a)

    - Laser assisted hopping

2. Model (b)

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

    (quantum Brownian motion) supplemented by a colored

    non-Markovian classical noise

3. Model (c)

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

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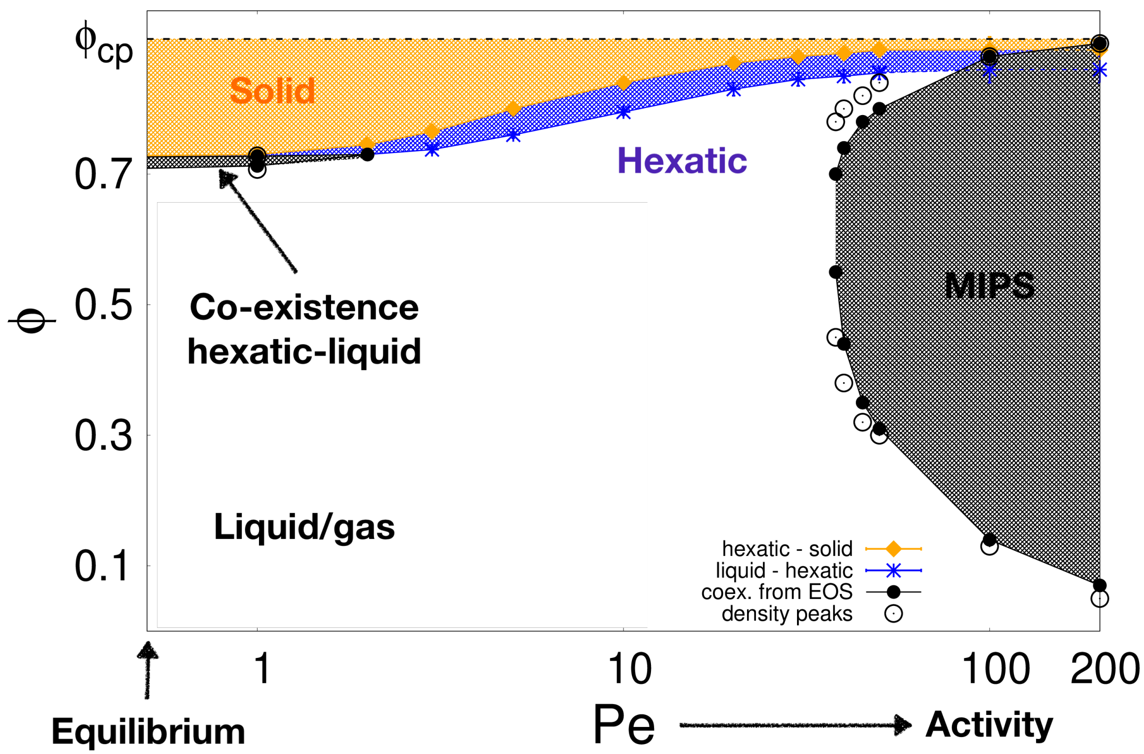
Perspectives

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)