Self-propelled particles as an active matter system

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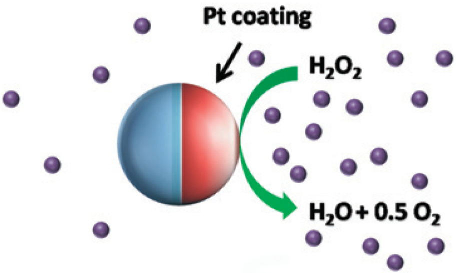
Open Statistical Physics

The Open University

Introduction

Active matter: interacting self-propelled particles

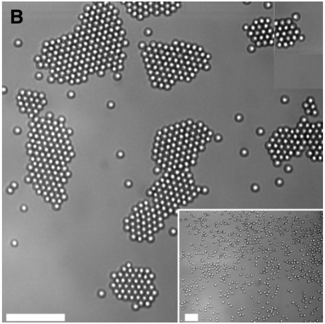
Janus particle



A. Walther and A. H. E. Müller, Soft Matter **4**, 663 (2008)

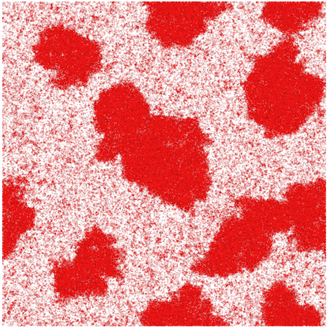
Introduction

Light-induced clusters of colloids



J. Palacci *et al.*, Science **339**, 936 (2013)

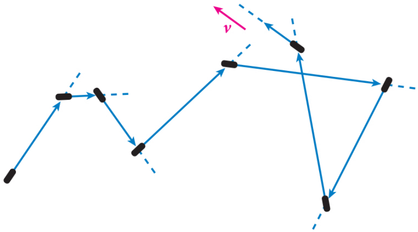
Simulated interacting active colloids



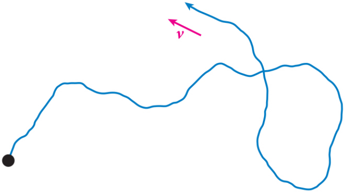
G. S. Redner *et al.*,
Phys. Rev. Lett. **110**, 055701 (2013)

Introduction

Run-and-tumble particles



Active Brownian particles



M. E . Cates and J. Tailleur, Ann. Rev. CMP **6**, 219 (2015)

Introduction

Many-body dynamics

$$0 = -\nabla_i U - \frac{\mathrm{d}x_i}{\mathrm{d}t} + \xi_i$$

Equilibrium fluctuations ξ_i

$$\langle \xi_i(t)\xi_j(0)\rangle \equiv 2T\delta_{ij}\delta(t)$$

No memory and Gaussian

Boltzmann steady-state

$$P_{\mathrm{s}} \sim \mathrm{e}^{-U/T}$$

Introduction

Many-body dynamics

$$0 = -\nabla_i U - \frac{\mathrm{d}x_i}{\mathrm{d}t} + v_i$$

Nonequilibrium self-propulsion v_i

$$\langle v_i(t) v_j(0) \rangle \equiv T \delta_{ij} \frac{\mathrm{e}^{-|t|/\tau}}{\tau}$$

Memory and non-Gaussian

Non-Boltzmann steady-state

Main questions of interest

- Phase diagram: equilibrium mapping

  J. Tailleur *et al.*, Phys. Rev. Lett. **100**, 218103 (2008)

- Equation of state: pressure vs. density

  A. P. Solon *at al.*, Phys. Rev. Lett. **114**, 198301 (2015)

How far from equilibrium is active matter?

Outline

1. Interacting active particles
   - Minimal model of self-propulsion
   - Effective equilibrium regime

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2. Active field theory
   - Coarse-grained dynamics
   - Spatial structure of nonequilibrium

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Interacting active particles

Many-body dynamics

$$0 = -\nabla_i U - \frac{\mathrm{d}x_i}{\mathrm{d}t} + v_i$$

Nonequilibrium self-propulsion v_i

Memory and Gaussian

C. Maggi *et al.*, Sci. Rep. **5**, 10724 (2015)

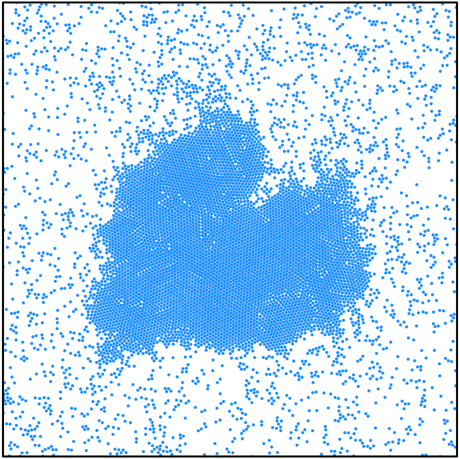
T. F. F. Farage *et al.*, Phys. Rev. E **91**, 042310 (2015)

Control parameter = Persistence time τ

Equilibrium for $\tau \to 0$

Interacting active particles

Interacting repulsive particles



ÉF *et al.*, Phys. Rev. Lett. **117**, 038103 (2016)

Interacting active particles

Comparing forward and backward dynamics

Quantifying irreversibility

$$\mathcal{S} \equiv \lim_{t\to\infty} \frac{1}{t} \ln \frac{\mathcal{P}}{\mathcal{P}^{\mathsf{R}}}$$

Entropy production rate

Equilibrium limit $\mathcal{S} \underset{\tau=0}{=} 0$

Interacting active particles

Passive Brownian particles + non-conservative force F_i

$$\mathcal{S} = \frac{\left\langle F_i \frac{\mathrm{d}x_i}{\mathrm{d}t} \right\rangle}{T} = \frac{\text{power of } F_i}{\text{temperature}}$$

Self-propelled particles

$$\mathcal{S} = \frac{\tau^2}{2T} \left\langle \nabla_i^3 U \left(\frac{\mathrm{d}x_i}{\mathrm{d}t} \right)^3 \right\rangle$$

Interacting active particles

Perturbative treatment in $\mathrm{Pe} \equiv \sqrt{\frac{\text{persistence time}}{\text{relaxation time}}}$

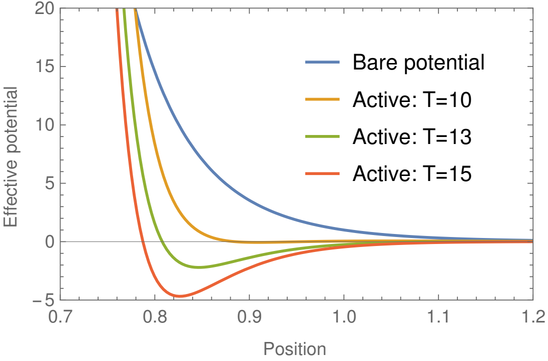
- $P_\mathrm{S} \sim \mathrm{e}^{-U/T} \left[1 + \mathcal{O}\left(\mathrm{Pe}^2\right)\right]$
- $\left\langle \nabla_i^3 U \left(\frac{\mathrm{d}x_i}{\mathrm{d}t}\right)^3 \right\rangle = \mathcal{O}\left(\mathrm{Pe}^3\right)$

$$\text{Effective equilibrium regime} \begin{cases} \text{Non-Boltzmann statistics} \\ \text{Time reversal symmetry} \end{cases}$$

Interacting active particles

Effective potential

$$U_{\text{eff}} \equiv U + \tau \left[\frac{(\nabla_i U)^2}{2} - T \nabla_i^2 U \right]$$



Original pair-wise potential

$$U \equiv \frac{1}{2} \sum_{\{i,j\}=1}^{N} V(r_i - r_j)$$

$$V \sim \frac{1}{x^{12}}$$

Interacting active particles

External perturbation $f_i(t)$

$$\langle \delta x_i(t) \rangle \equiv \int_0^t R(t-s) f_i(s) \mathrm{d}s$$

Response function $R(t)$

Passive Brownian particles

$$R(t) \underset{\tau=0}{=} -\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}t} \langle x_i(t) x_i(0) \rangle$$

Fluctuation-dissipation theorem

Interacting active particles

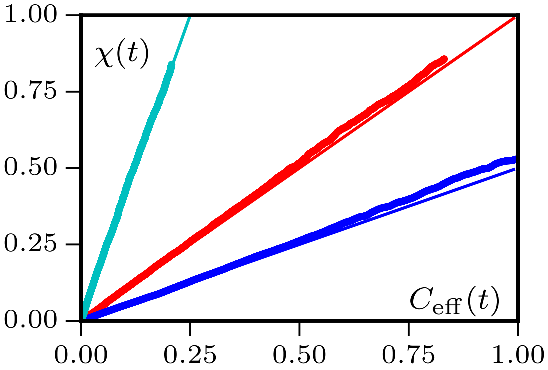
Fluctuation-dissipation relation

$$R(t) = -\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle x_i(t)x_i(0) + \tau^2 \frac{\mathrm{d}x_i(t)}{\mathrm{d}t}\frac{\mathrm{d}x_i(0)}{\mathrm{d}t}\right\rangle$$

Probing effective equilibrium regime

Interacting active particles

Numerical simulations: 3 values of T



Susceptibility

$$\chi(t) \equiv \frac{1}{N}\int_0^t R(t-s)\mathrm{d}s$$

Correlation

$$C_{\rm eff}(t) \equiv \frac{1}{N}\left\langle x_i^2(t) + \tau^2 \left[\frac{\mathrm{d}x_i(t)}{\mathrm{d}t}\right]^2\right\rangle - \frac{1}{N}\left\langle x_i(t)x_i(0) + \tau^2 \frac{\mathrm{d}x_i(t)}{\mathrm{d}t}\frac{\mathrm{d}x_i(0)}{\mathrm{d}t}\right\rangle$$

Outline

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   - Minimal model of self-propulsion
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2. Active field theory
   - Coarse-grained dynamics
   - Spatial structure of nonequilibrium

Active field theory

Fluctuating density field

$$\rho(x,t) \equiv \sum_{i=1}^{N} \delta\left[x - x_i(t)\right]$$

Active model B

$$\phi \equiv \delta\rho/\rho_0 \;\rightarrow\; \partial_t \phi = \nabla\left[\nabla\left(\frac{\delta\mathcal{F}}{\delta\phi} + \mu_{\mathrm{A}}\right) + \Lambda\right]$$

Equilibrium fluctuations Λ

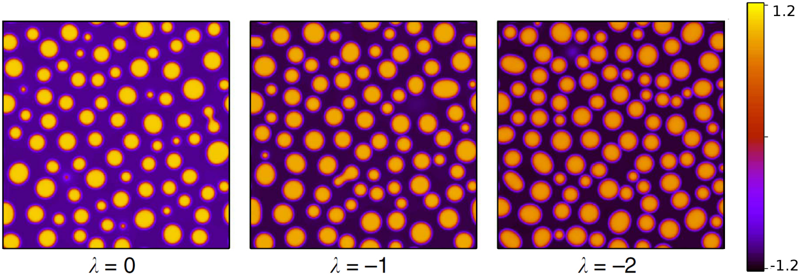
Active chemical potential μ_{A}

Active field theory

Phase separation

$$\mathcal{F} \equiv \int \left[\frac{a}{2}\phi^2 + \frac{b}{4}\phi^4 + \frac{\kappa}{2} |\nabla\phi|^2 \right] \mathrm{d}x$$

Active chemical potential $\mu_{\rm A} \equiv \lambda |\nabla\phi|^2$



R. Wittkowski *et al.*, Nat. Com. **5**, 4351 (2014)

Active field theory

Entropy production rate

$$\mathcal{S} = \frac{1}{T} \int \langle \mu_{\mathrm{A}} \partial_t \phi \rangle \, \mathrm{d}x \equiv \int \sigma(x) \, \mathrm{d}x$$

Spatial density of entropy production

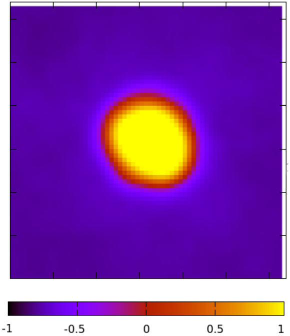
$$\sigma = \frac{\lambda}{T} \left\langle |\nabla \phi|^2 \, \partial_t \phi \right\rangle$$

Probing nonequilibrium from field profile

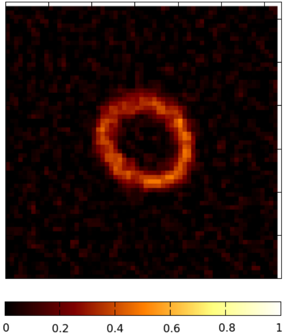
Active field theory

Spatial structure of entropy production rate

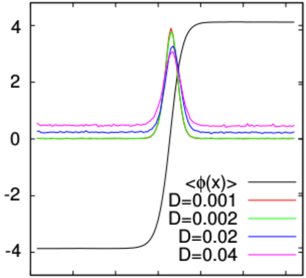
Field profile



Entropy density



Entropy density



C. Nardini *et al.*, Phys. Rev. X (2017)

Active field theory

External perturbation $h(x,t)$

$$\langle \delta\phi(x,t)\rangle \equiv \int R_\phi(x-y,t-s)h(y,s)\mathrm{d}y\mathrm{d}s$$

Response function $R_\phi(x,t)$

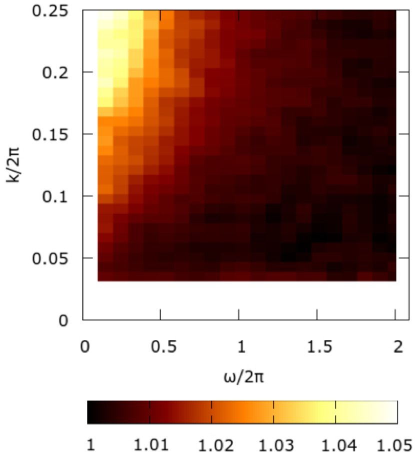
Equilibrium dynamics

$$R_\phi(x-y,t) \underset{\mu_\mathrm{A}=0}{=} -\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}t}\langle \phi(x,t)\phi(y,0)\rangle$$

Fluctuation-dissipation theorem

Violation of fluctuation-dissipation

$\omega C(k,\omega)/2TR_\phi(k,\omega)$



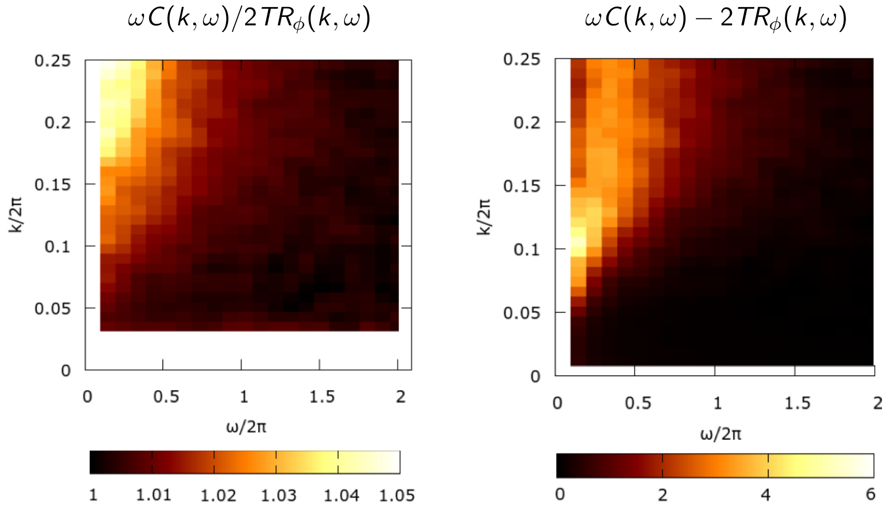
Response

$$R_\phi(k,\omega) \equiv \int R_\phi(x,t) e^{ikx} \sin(\omega t) dt dx$$

Correlation

$$C(k,\omega) \equiv \int \langle \phi(x,t)\phi(0,0) \rangle \, e^{i(kx+\omega t)} dt dx$$

Violation of fluctuation-dissipation



Active field theory

Spectral decomposition of entropy production

$$\mathcal{S} \equiv \int \sigma_\phi(k,\omega)\frac{\mathrm{d}k\mathrm{d}\omega}{(2\pi)^{d+1}}$$

Generalized Harada-Sasa relation

$$\sigma_\phi(k,\omega) = \frac{\omega}{Tk^2}\Big[\omega C(k,\omega) - 2TR_\phi(k,\omega)\Big]$$

Violation of fluctuation-dissipation

Conclusion

Nonequilibrium properties of active systems

- Interacting active particles

  Effective equilibrium regime

- Active field theory

  Spatial structure of nonequilibrium

References: Phys. Rev. Lett. **117**, 038103 (2016) | `arXiv:1604.00953`

Phys. Rev. X (2017) | `arXiv:1610.06112`