Self-propelled particles as an active matter system

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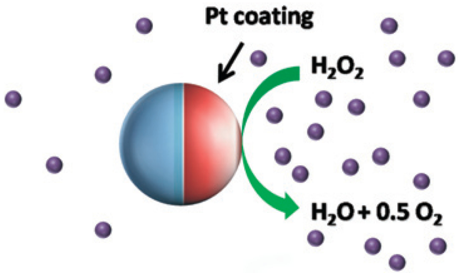
Active matter: interacting self-propelled particles

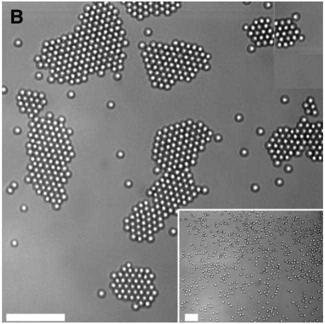
Janus particle



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

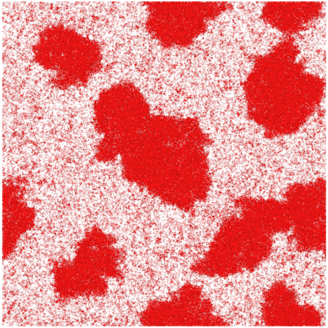
Introduction

Light-induced clusters of colloids



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

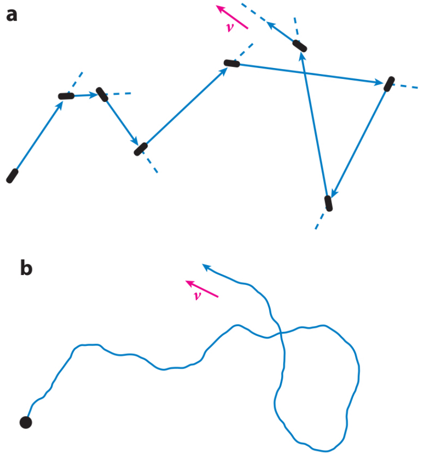
Simulated interacting active colloids



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

Introduction

Run-and-tumble and active Brownian particles



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

Introduction

Many-body dynamics

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

Equilibrium fluctuations ξ_i

No memory and Gaussian

Boltzmann distribution

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

Introduction

Many-body dynamics

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

Nonequilibrium self-propulsion v_i

Memory and non-Gaussian

Non-Boltzmann distribution

Main questions of interest

- Phase diagram: equilibrium mapping

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

- Equation of state: pressure

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

- Nonequilibrium properties

Outline

1. Interacting active particles
   - Minimal model of self-propulsion
   - How far from equilibrium?
   - 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

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

Nonequilibrium self-propulsion v_i

Memory and Gaussian

G. Szamel et al., Phys. Rev. E **91**, 062304 (2015)

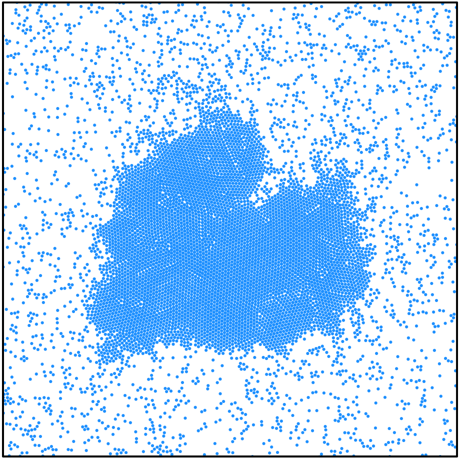
C. Maggi *et al.*, Sci. Rep. **5**, 10724 (2015)

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

Persistence time τ $\rightarrow$ Equilibrium $\tau = 0$

Interacting active particles

Interacting repulsive particles



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

Comparing forward and backward dynamics

Quantifying irreversibility

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

Entropy production rate

Equilibrium $\quad \mathcal{S} = 0$

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

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

Interacting active particles

Péclet number

$$\mathrm{Pe} = \frac{\text{persistence length}}{\text{interaction range}}$$

$$\mathrm{Pe} = \sqrt{\frac{\text{persistence time}}{\text{relaxation time}}}$$

Competition self-propulsion/interaction

Interacting active particles

Perturbative treatment in Péclet number

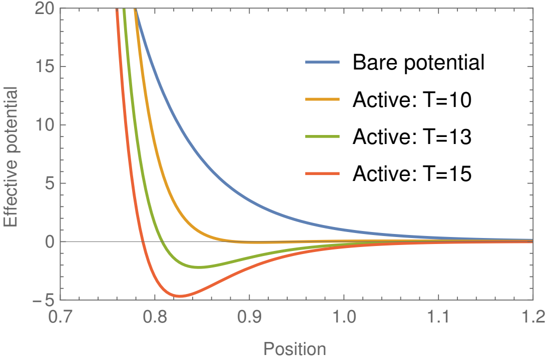
- $P_{\mathrm{S}} \sim \mathrm{e}^{-U/T} \left[1 + \mathcal{O}\left(\mathrm{Pe}^2\right)\right]$
- $\left\langle \nabla_i^3 U \left(\frac{\mathrm{d}x_i}{\mathrm{d}t}\right)^3 \right\rangle = \mathcal{O}\left(\mathrm{Pe}^3\right)$

Effective equilibrium regime $\left\{ \begin{array}{l} \text{Non-Boltzmann statistics} \\ \text{Time reversal symmetry} \end{array} \right.$

Interacting active particles

Effective potential

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



Original pair-wise potential

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

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

Interacting active particles

External perturbation $f_i(t)$

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

Response function $R(t)$

Passive Brownian particles

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

Fluctuation-dissipation theorem

Interacting active particles

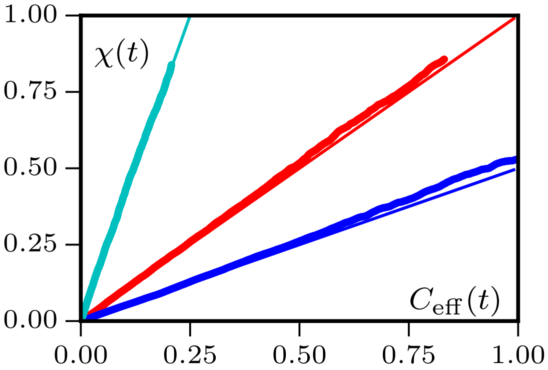
Fluctuation-dissipation relation

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

Probing effective equilibrium

Interacting active particles

Numerical simulations: 3 values of T



Susceptibility

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

Correlation

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

Outline

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Active field theory

Fluctuating density field

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

Active model B

$$\partial_t \rho = \nabla \left[\nabla \left(\frac{\delta \mathcal{F}}{\delta \rho} + \mu_{\mathsf{A}} \right) + \Lambda \right]$$

Equilibrium fluctuations Λ

Active chemical potential μ_{A}

Active field theory

Phase separation

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

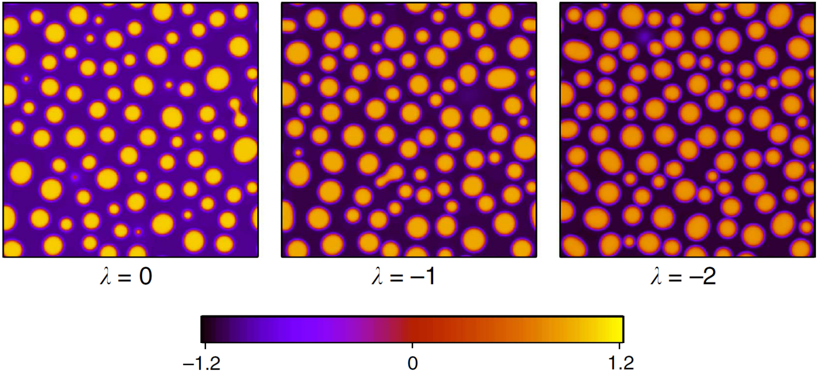
Cahn-Hilliard free energy

Active chemical potential

$$\mu_{\mathsf{A}} = \lambda |\nabla \rho|^2$$

Active field theory

Shift of coexisting phase densities



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

Active field theory

Entropy production rate

$$\mathcal{S} = \frac{1}{T} \int \left\langle \mu_{\mathsf{A}} \partial_t \rho \right\rangle \mathrm{d}x$$

Spatial density of entropy production

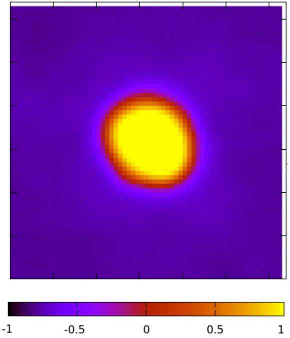
$$\sigma = \frac{\lambda}{T} \left\langle \, |\nabla \rho|^2 \, \partial_t \rho \right\rangle$$

Probing nonequilibrium from field profile

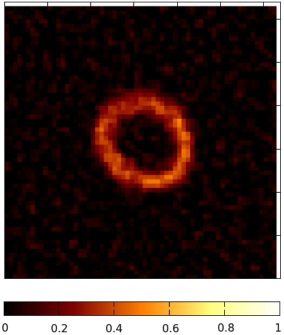
Active field theory

Spatial structure of entropy production rate

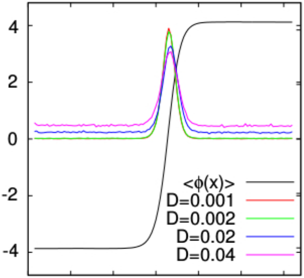
Field profile



Entropy density



Entropy density



C. Nardini *et al.*, `arXiv:1610.06112`

Active field theory

External perturbation $h(x,t)$

$$\langle \delta\rho(x,t) \rangle = \int R(x-y, t-s) h(y,s) \mathrm{d}y \mathrm{d}s$$

Response function $R(x,t)$

Equilibrium dynamics

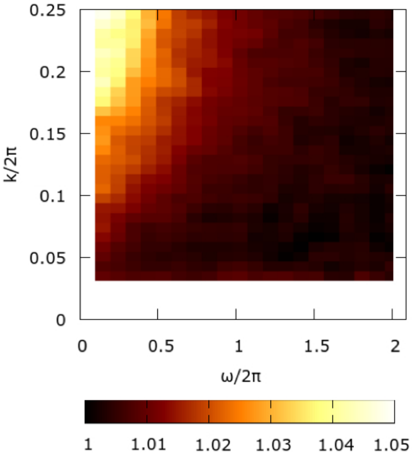
$$R(x-y,t) = -\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}t} \langle \rho(x,t)\rho(y,0) \rangle$$

Fluctuation-dissipation theorem

Active field theory

Violation of fluctuation-dissipation

$\omega C(k,\omega)/2TR(k,\omega)$



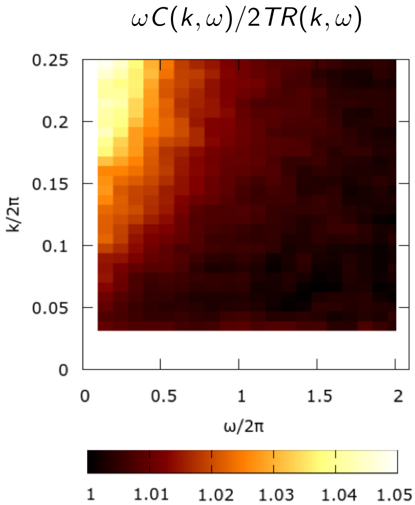
Response

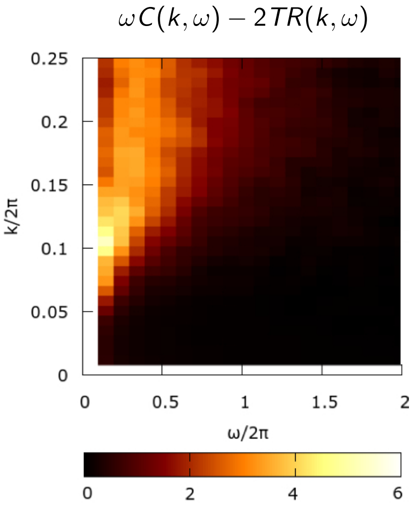
$$R(k,\omega) = \int R(x,t)\mathrm{e}^{\mathrm{i}kx}\sin(\omega t)\mathrm{d}t\mathrm{d}x$$

Correlation

$$C(k,\omega) = \int \langle\rho(x,t)\rho(0,0)\rangle\,\mathrm{e}^{\mathrm{i}(kx+\omega t)}\mathrm{d}t\mathrm{d}x$$

Violation of fluctuation-dissipation





Active field theory

Spectral decomposition of entropy production

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

Violation of fluctuation-dissipation

$$\sigma(k,\omega) = \frac{\omega}{Tk^2}\left[\omega C(k,\omega) - 2TR(k,\omega)\right]$$

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:1610.06112

Conclusion

Future directions

- Other models of self-propulsion

  Non-Gaussian without memory

- Hydrodynamic description

  Dynamics of passive tracer

Interacting active particle

Density waves around an obstacle