Self-propelled particles as an active matter system

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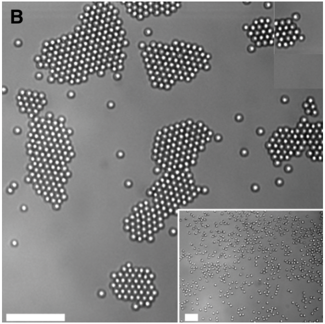
Introduction

Light-induced clusters of colloids



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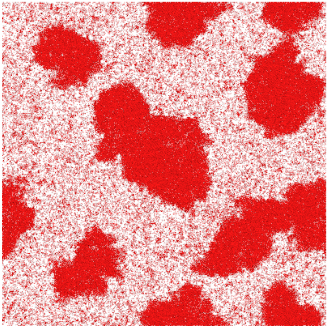
Simulated interacting active colloids



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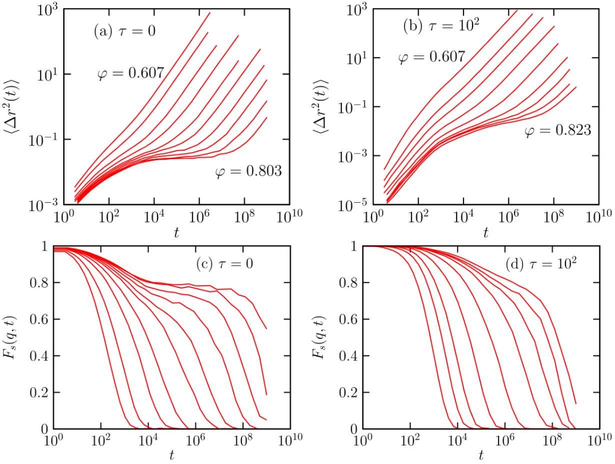
Dense suspension of active colloids: glassy dynamics



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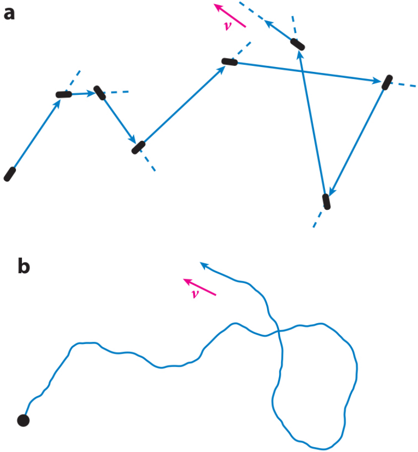
Introduction

Run-and-tumble and active Brownian particles



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Introduction

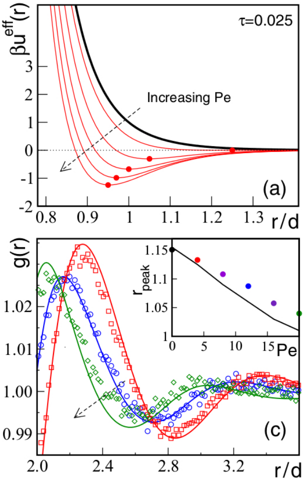
Competition self-propulsion/interaction

Péclet number

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

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

Introduction



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Introduction

Brownian particles

$$\gamma \dot{\mathbf{r}}_i = -\sum_j \nabla_i \phi(\mathbf{r}_i - \mathbf{r}_j) + \boldsymbol{\xi}_i$$

Mobility $\quad \mu = \gamma^{-1}$

Equilibrium fluctuations

$$\left\langle \boldsymbol{\xi}_i(t) \boldsymbol{\xi}_j(0) \right\rangle = 2\gamma T \delta_{ij} \delta(t)$$

$$P_{\mathrm{S}} = \exp\left[-\frac{1}{2T} \sum_{i,j} \phi(\mathbf{r}_i - \mathbf{r}_j) \right]$$

Introduction

Self-propelled particles

$$\dot{\mathbf{r}}_i = -\mu \sum_j \nabla_i \phi \left(\mathbf{r}_i - \mathbf{r}_j \right) + \mathbf{v}_i$$

Nonequilibrium fluctuations $\mathbf{v}$

- Random direction with fixed norm
- Memory and non-Gaussian

Main questions of interest

- Equation of state: temperature, pressure
- Phase diagram: stationary measure
- Structural relaxation: time scales

Outline

1. Searching for a minimal model of self-propulsion

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2. Quantifying nonequilibrium

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2. Quantifying nonequilibrium
3. Effective equilibrium regime

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Searching for a minimal model of self-propulsion

Overdamped dynamics

$$\dot{\mathbf{r}}_i = -\mu \nabla_i U + \mathbf{v}_i$$

External potential + pair-wise interactions

$$U = \sum_i V_{\text{ext}}(\mathbf{r}_i) + \frac{1}{2} \sum_{i,j} \phi(\mathbf{r}_i - \mathbf{r}_j)$$

Searching for a minimal model of self-propulsion

Overdamped dynamics

$$\dot{\mathbf{r}}_i = -\mu \nabla_i U + \mathbf{v}_i$$

Gaussian fluctuations

$$\langle \mathbf{v}_i(t) \mathbf{v}_j(0) \rangle = \delta_{ij} \frac{\mu T}{\tau} \mathrm{e}^{-|t|/\tau}$$

Equilibrium reference

$$\langle \mathbf{v}_i(t) \mathbf{v}_j(0) \rangle \underset{\tau \to 0}{\longrightarrow} 2\mu T \delta_{ij} \delta(t)$$

Searching for a minimal model of self-propulsion

No interaction: harmonic oscillator

$$\dot{r} = -\kappa\mu r + v$$

$$\langle v(t)v(0)\rangle = \frac{\mu T}{\tau} \mathrm{e}^{-|t|/\tau}$$

Stationary distribution

$$P_{\mathrm{S}} = \exp\left[-\left(1+\tau\kappa\mu\right)\frac{\kappa r^2}{2T}\right]$$

Searching for a minimal model of self-propulsion

No interaction: harmonic oscillator

$$\dot{r} = -\kappa\mu r + v$$

$$\langle v(t)v(0)\rangle = \frac{\mu T}{\tau} \mathrm{e}^{-|t|/\tau}$$

Stationary distribution

$$P_{\mathrm{s}} = \exp\left[-\left(1 + \mathrm{Pe}^2\right)\frac{\kappa r^2}{2T}\right]$$

Searching for a minimal model of self-propulsion

No interaction: harmonic oscillator

$$\dot{r} = -\kappa\mu r + v$$

$$\dot{v} = -\frac{v}{\tau} + \xi$$

$$\langle \xi(t)\xi(0)\rangle = \frac{2\mu T}{\tau^2}\delta(t)$$

Equilibrium underdamped dynamics

$$\dot{r} = p$$

$$\dot{p} = -\frac{p}{\tau} - \frac{\mu\kappa}{\tau}\left(1 + \frac{\kappa\tau}{\gamma}\right) r + \xi$$

Searching for a minimal model of self-propulsion

Interacting particles

$$\dot{r}_i = -\mu \nabla_i U + v_i$$

$$\dot{v}_i = -\frac{v_i}{\tau} + \xi_i$$

$$\langle \xi_i(t) \xi_j(0) \rangle = \frac{2\mu T}{\tau^2} \delta_{ij} \delta(t)$$

Nonequilibrium underdamped dynamics

$$\dot{r}_i = p_i$$

$$\dot{p}_i = -\frac{p_i}{\tau} - \mu p_k \partial^2_{ik} U - \frac{\mu}{\tau} \nabla_i U + \xi_i$$

Searching for a minimal model of self-propulsion

Previous attempt: neglecting inertia

$$\dot{r}_i = p_i$$

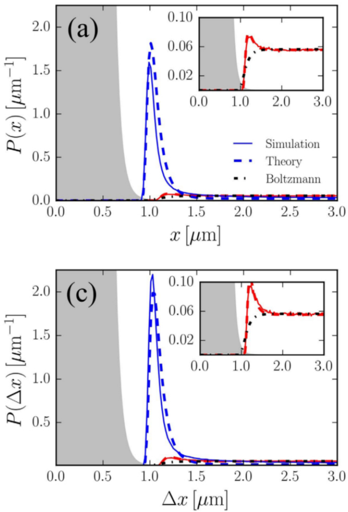
$$\cancel{\dot{p}_i} = -\frac{p_i}{\tau} - \mu p_k \partial^2_{ik} U - \frac{\mu}{\tau} \nabla_i U + \xi_i$$

Stationary measure

$$P_{\mathrm{S}} = \exp\left[-\frac{U}{T} - \frac{\tau^2}{2T} \left(\partial_i U\right)^2\right] |\det \mathbb{M}|$$

$$\mathbb{M}_{ij} = \delta_{ij} + \tau\mu\partial^2_{ij} U$$

Searching for a minimal model of self-propulsion



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Searching for a minimal model of self-propulsion

Previous attempt: neglecting inertia

$$\dot{r}_i = p_i$$

$$\cancel{\dot{p}_i} = -\frac{p_i}{\tau} - \mu p_k \partial^2_{ik} U - \frac{\mu}{\tau} \nabla_i U + \xi_i$$

Mapping to equilibrium dynamics

Outline

1 Searching for a minimal model of self-propulsion

2 Quantifying nonequilibrium

3 Effective equilibrium regime

Quantifying nonequilibrium

Entropy production rate

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

Brownian particles + non-conservative force

$$\gamma \dot{r}_i = F_i - \partial_i U + \xi_i$$

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

$$\sigma = \frac{1}{T} \langle \dot{r}_i F_i \rangle$$

Quantifying nonequilibrium

Self-propelled particles

$$\dot{r}_i = -\mu\partial_i U + v_i$$

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

Entropy production

$$\sigma = \frac{\tau^2}{2T}\sum_{ijk}\left\langle \dot{r}_i\dot{r}_j\dot{r}_k\partial^3_{ijk}U\right\rangle$$

Quantifying nonequilibrium

Péclet number

$$\mathrm{Pe} = \frac{\text{persistence length}}{\text{interaction range}} = \sqrt{\frac{\tau}{\tau_\mathrm{R}}}$$

Relaxation time

$$\tau_\mathrm{R} = \frac{(\text{interaction range})^2}{\mu T}$$

Quantifying nonequilibrium

Self-propelled particles: scaled dynamics

- space unit $=$ interaction range
- time unit $= \tau/\mathrm{Pe}$
- energy unit $= T$

Quantifying nonequilibrium

Self-propelled particles: scaled dynamics

$$\dot{r}_i = p_i$$

$$\dot{p}_i = -\frac{1}{\mathrm{Pe}}\left(p_i + \mathrm{Pe}^2 p_j \partial^2_{ij} U\right) - \partial_i U + \xi_i$$

$$\langle \xi_i(t) \xi_i(0) \rangle = \frac{2}{\mathrm{Pe}} \delta_{ij} \delta(t)$$

Quantifying nonequilibrium

Self-propelled particles: scaled dynamics

$$\dot{r}_i = p_i$$

$$\dot{p}_i = -\frac{1}{\mathrm{Pe}}\left(p_i + \mathrm{Pe}^2 p_j \partial_{ij}^2 U\right) - \partial_i U + \xi_i$$

$$\langle \xi_i(t)\xi_i(0)\rangle = \frac{2}{\mathrm{Pe}}\delta_{ij}\delta(t)$$

Maggi *et al.*: Pe finite and $\mathrm{Pe} \to 0$

Quantifying nonequilibrium

Entropy production

$$\sigma = \frac{\mathrm{Pe}^2}{2} \sum_{ijk} \left\langle p_i p_j p_k \partial^3_{ijk} U \right\rangle$$

Small Pe expansion

$$\sum_{ijk} \left\langle p_i p_j p_k \partial^3_{ijk} U \right\rangle = c_1 \mathrm{Pe} + c_2 \mathrm{Pe}^2 + c_3 \mathrm{Pe}^3 + \mathcal{O}\left(\mathrm{Pe}^4\right)$$

Quantifying nonequilibrium

Stationary measure

$$P_{\mathrm{S}} = \mathrm{e}^{-U - \frac{p_i^2}{2}} \left\{ 1 - \frac{\mathrm{Pe}^2}{2} \left[(\partial_i U)^2 + \mathcal{L} U \right] + \frac{\mathrm{Pe}^3}{6} p_i \partial_i \mathcal{L} U + \mathcal{O}\left(\mathrm{Pe}^4\right) \right\}$$

$$\mathcal{L} U = (p_j p_k - 3\delta_{jk}) \partial_{jk}^2 U$$

- Position-velocity coupling
- Term Pe^3 odd in velocity

Quantifying nonequilibrium

Entropy production

$$\sigma = \frac{\mathrm{Pe}^5}{2\mathcal{Z}} \int_r \left(\partial^3_{ijk} U\right)^2 \mathrm{e}^{-U} + \mathcal{O}\left(\mathrm{Pe}^6\right)$$

No contribution from the Pe^2 term of the measure

Outline

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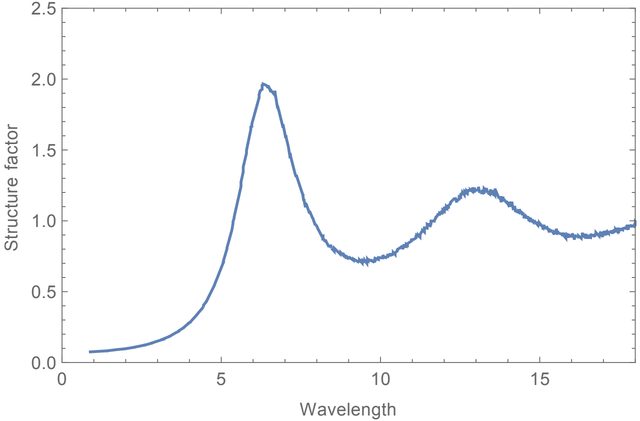
Effective equilibrium regime

Stationary distribution

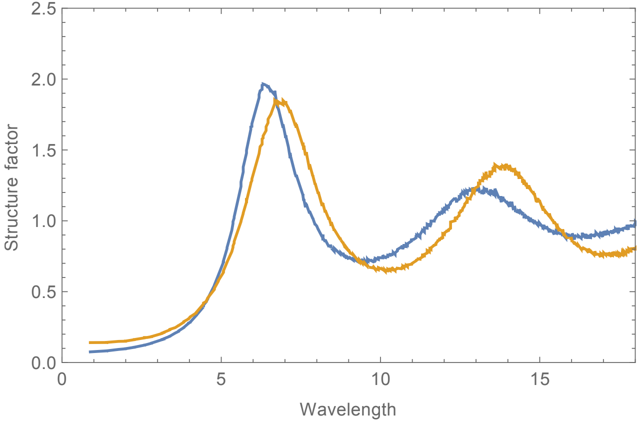
$$P_{\mathrm{S}} = \exp\left\{ -U - \mathrm{Pe}^2 \left[\frac{(\partial_i U)^2}{2} - \partial_{ii}^2 U \right] + \mathcal{O}\left(\mathrm{Pe}^4\right) \right\}$$

- Three-body interactions
- Attractive effects from bare repulsion

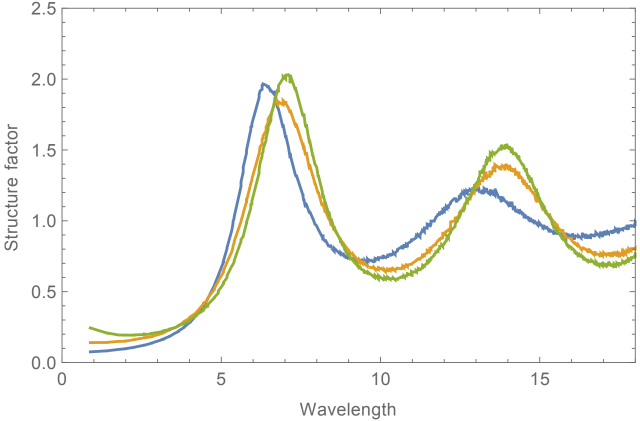
Effective equilibrium regime



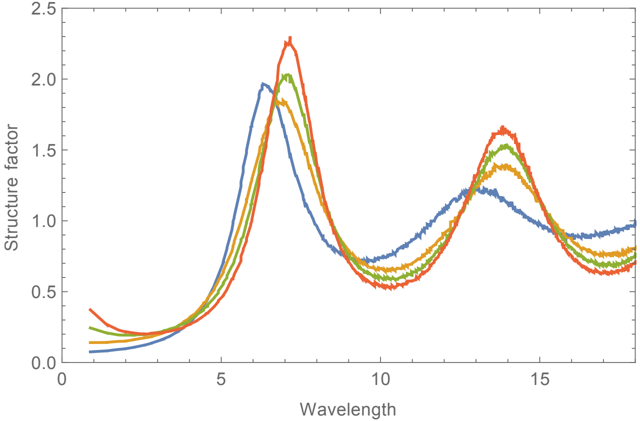
Effective equilibrium regime



Effective equilibrium regime



Effective equilibrium regime



Effective equilibrium regime

Brownian particles: external perturbation

$$\gamma \dot{r}_i = f_i - \partial_i U + \xi_i$$

Response function

$$R(t) = \left. \frac{\delta \langle r_i(t) \rangle}{\delta f_i(0)} \right|_{f=0}$$

Fluctuation-dissipation theorem

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

Effective equilibrium regime

Self-propelled particles: external perturbation

$$\dot{r}_i = \mu\left(f_i - \partial_i U\right) + v_i$$

Scaled dynamics

$$\dot{p}_i = -\frac{1}{\mathrm{Pe}}\left(p_i + \mathrm{Pe}^2 p_j \partial_{ij}^2 U\right) + f_i + \mathrm{Pe}\dot{f}_i - \partial_i U + \xi_i$$

$$\langle \xi_i(t)\xi_i(0)\rangle = \frac{2}{\mathrm{Pe}}\delta_{ij}\delta(t)$$

Effective equilibrium regime

Fluctuation-dissipation relation with Pe $= 0$

$$R(t) = -\frac{\mathrm{d}}{\mathrm{d}t} \underbrace{\left[\langle r_i(t) r_i(0) \rangle + \mathrm{Pe}^2 \langle \dot{r}_i(t) \dot{r}_i(0) \rangle \right]}_{C(t)}$$

Susceptibility $\quad \chi(t) = \int_0^t R(s)\mathrm{d}s$

Correlation $\quad \Delta C(t) = C(0) - C(t)$

Effective equilibrium regime

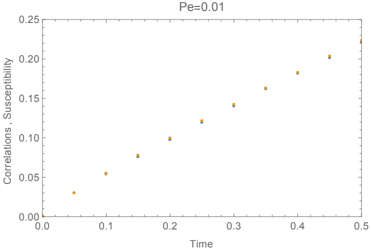
Fluctuation-dissipation relation when $\mathrm{Pe} \to 0$

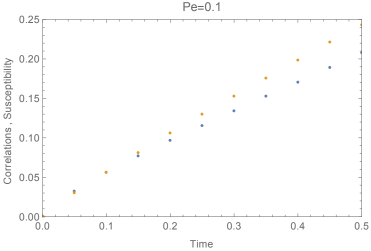
$$R(t) = -\frac{\mathrm{d}}{\mathrm{d}t} \underbrace{\left[\langle r_i(t) r_i(0) \rangle + \mathrm{Pe}^2 \langle \dot{r}_i(t) \dot{r}_i(0) \rangle \right]}_{C(t)} + \mathcal{O}\left(\mathrm{Pe}^4\right)$$

Susceptibility $\quad \chi(t) = \int_0^t R(s) \mathrm{d}s$

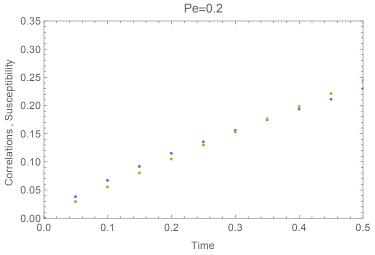
Correlation $\quad \Delta C(t) = C(0) - C(t)$

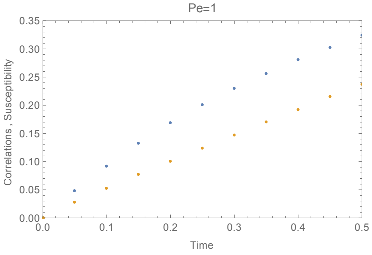
Effective equilibrium regime





Effective equilibrium regime





Conclusion

Minimal model of self-propulsion

Gaussian exponentially correlated fluctuations

- Stationary measure in position-velocity
- Entropy production
- Fluctuation dissipation relation

Outlook

Future directions

- Collective modes

  Hydrodynamic equations, tracer dynamics

- Non-Gaussian white fluctuations | H. Hayakawa

  Static structure, phase separation