A Particle-Scale Continuum Model for Active Brownian Particles

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Active Brownian particles (ABPs)

Active Brownian Particles (ABPs), consisting of Brownian particles driven by a constant self-propulsion force in an overdamped environment. The fundamental distinction between ABPs and traditional Brownian particles lies in the intrinsic orientation of the former, which breaks the isotropy inherent in standard Brownian motion. This broken symmetry allows ABPs to exhibit unique **elastic properties**. To capture these emergent behaviors, we aim to develop a **particle-scale continuum model** specifically for ABPs

$$\dot{\boldsymbol{r}}_i(t) = v_A\hat{u}(\phi_i) + \boldsymbol{v}_{int,i}(\{\mathbf{r}_j\}) + \sqrt{2D_T}\boldsymbol{\Lambda}_{T,i} \qquad Pe = \frac{v_A\sigma}{D_T}$$

$$\dot{\phi}_i = \sqrt{2D_R}\Lambda_{R,i}(t) \qquad \Phi = \frac{N\pi\sigma^2}{4L^2}$$

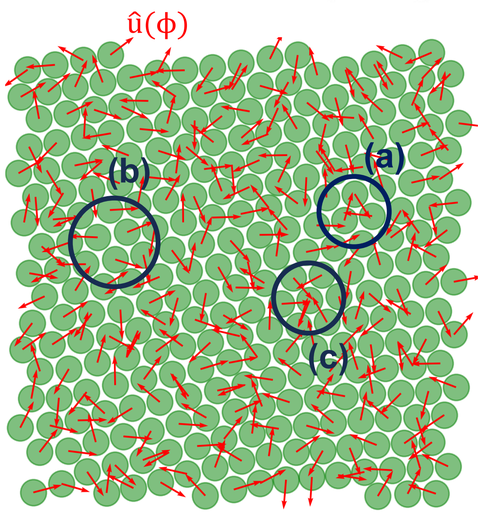


Fig. 1: MD simulation with $Pe = 150,\ \Phi = 0.5$. Self-propelled orientations (red arrows) breaks rotational symmetry of the elastic response of lattices. Take the following sites for example.
(a) $\nabla\times\hat{u} < 0$, asymmetric shear response is expected.
(b) $\nabla\cdot\hat{u} > 0$, easier to compress locally
(c) $\nabla\cdot\hat{u} < 0$, more difficult to compress locally

Phase Field Crystal (PFC) Like Model?

PFC is a **particle-scale** continuum field theory that describes particles with a osciilating density field, which gives rise to elasticity. **We aim to develop a particle-scale mean field theory for ABPs that captures intricate interactions between the density field and the polarization field**, which sheds light on the polarization-dependent elastic response of active systems.

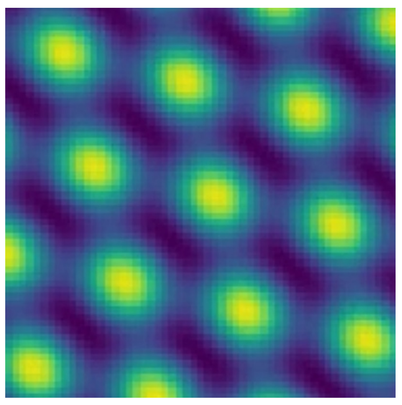


Fig. 2: Density field profile of APFC

PFC model (Elder *et al.*, 2002)

$$\frac{\partial\rho(\mathbf{r},t)}{\partial t} = \nabla^2\frac{\delta F}{\delta\rho}$$

$$F[\rho(\mathbf{r})] = \int d\mathbf{r}\left[\frac{1}{2}\rho\left(-\epsilon + \left(1+\nabla^2\right)^2\right)\rho + \frac{1}{4}\rho^4\right]$$

Dynamical Density Functional Theory (DDFT)

We resort to DDFT to derive the continuum model, starting with the continuity equation.

$$\frac{\partial P(\mathbf{X})}{\partial t} = -\nabla\cdot\left(\frac{d\mathbf{X}}{dt}P\right) \qquad \boldsymbol{X} = (\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ldots,\phi_1,\ \phi_2,\ldots)$$

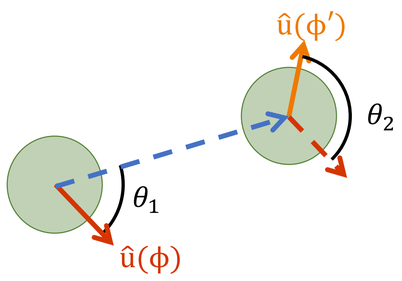
$$\dot{\rho}(\boldsymbol{r},\phi,t) = \left(D_T\nabla_r^2 + D_R\partial_\phi^2 - v_A\hat{\boldsymbol{u}}(\phi)\cdot\nabla_r\right)\rho(\boldsymbol{r},\phi,t)$$

$$-\beta D_T\nabla\cdot\left[\rho(\boldsymbol{r},\phi,t)\int \mathrm{d}^2\mathbf{r}'\,\mathrm{d}\phi'\nabla_{\vec{r}}U_2(|\boldsymbol{r}-\boldsymbol{r}'|)\rho(\boldsymbol{r}',\phi',t)g(\boldsymbol{r},\boldsymbol{r}',\phi,\phi')\right]$$

$$\rho(\vec{r},\phi) \approx \rho(\vec{r}) + \vec{P}(\vec{r})\cdot\hat{u}(\phi)$$

$$\rho(\vec{r}) = \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\phi\rho(\vec{r},\phi)$$

$$\vec{P}(\vec{r}) = \frac{1}{\pi}\int_0^{2\pi}\mathrm{d}\phi\rho(\vec{r},\phi)\hat{u}(\phi)$$



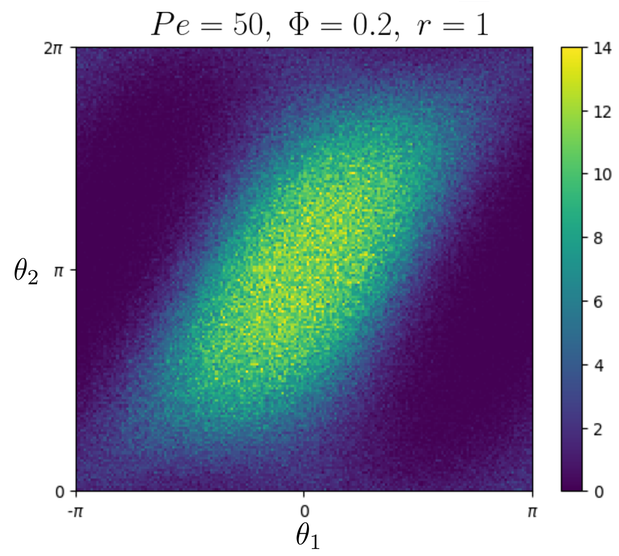


Fig. 3: Pair distribution function $g(r,\theta_1,\theta_2)$ obtained from molecular dynamics (MD) simulations by averaging the local neighbor distribution around each particle.

$$\dot{\rho} = D_T\nabla^2\rho - \frac{1}{2}v_A\nabla\cdot\vec{P} + \beta D_T\nabla\cdot\left\{A_1\rho\vec{P} + A_2\vec{\nabla}(\vec{P}^2) + A_3\rho\vec{\nabla}\rho + \ldots\right\}$$

$$\dot{\vec{P}} = D_T\nabla^2\vec{P} - D_R\vec{P} - v_A\vec{\nabla}\rho + \beta D_T\left\{A_{11}\vec{\nabla}\cdot((\vec{\nabla}\rho)\otimes\vec{P}) + A_{12}\vec{\nabla}\cdot(\rho\vec{\nabla}\otimes\vec{P}) + \ldots\right\}$$

Linear Stability Analysis

We add small perturbation to homogeneous state, $\rho(\vec{r}) = \bar{\rho} + \delta\rho,\ \vec{P} = \delta\vec{P}$, to examine its stability. If perturbation decays, the homogeneous state is stable; Otherwise, a preferred wavelength is selected, hence elasticity.

$$\delta\dot{\rho} = D_T\nabla^2\delta\rho - \frac{v_A}{2}\nabla\cdot\delta\vec{P} + \hat{L}_\rho(\delta\rho,\delta\vec{P})$$

$$\delta\dot{\vec{P}} = D_T\nabla^2\delta\vec{P} - D_R\delta\vec{P} - v_A\nabla\delta\rho + \hat{L}_{\vec{P}}(\delta\rho,\delta\vec{P})$$

$$\Rightarrow \quad \delta\rho = \sum_k\rho_k(t)e^{i\vec{k}\cdot\vec{r}}, \qquad \delta\vec{P} = \sum_k\vec{P}_k(t)e^{i\vec{k}\cdot\vec{r}}$$

$$\Rightarrow \quad \frac{d}{dt}\begin{bmatrix}\rho_k\\ \vec{P}_k\end{bmatrix} = \hat{A}(k)\begin{bmatrix}\rho_k\\ \vec{P}_k\end{bmatrix}$$

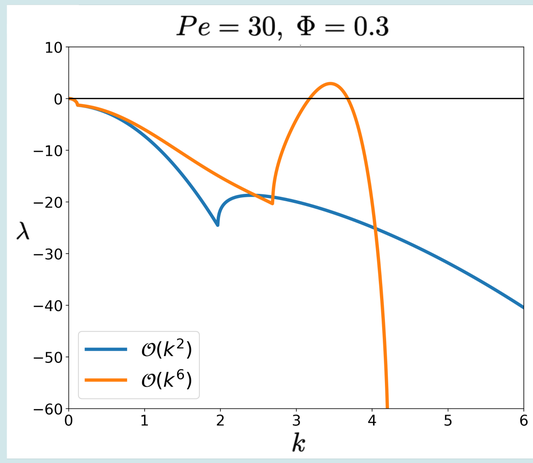


Fig. 4: The growth rate λ of perturbed plane waves of wavenumber *k*.

Phase diagram

The phase diagram of ABPs is constructed using the linear stability analysis. While most research employs **negative diffusion** (∇^2 or k^2 terms) as the criterion to determine the spinodal line, our extension to the dynamical equations of $\mathcal{O}(k^6)$ yields a **different phase boundary** (cyan dashed line). This suggests a window of new phases between the homogeneous and clustered states, bounded by the cyan dashed curve and the cluster phase.

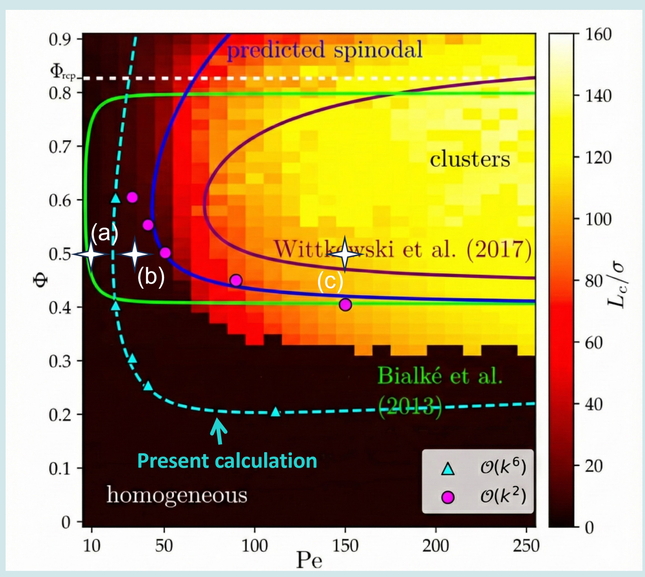


Fig. 5: Adapted from *J. Phys.: Condens. Matter* **35**, 313001 (2023).

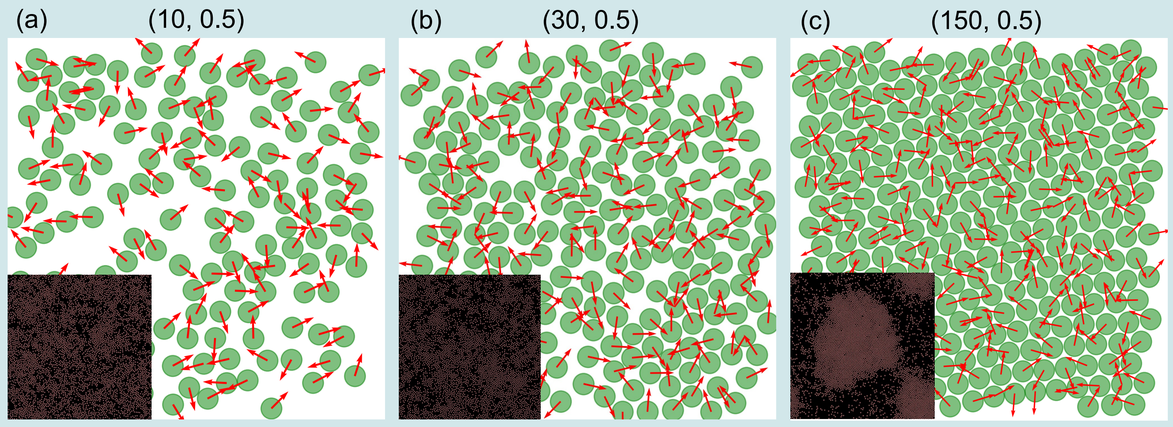


Fig. 6: Snapshots of MD simulations for the corresponding parameters (a), (b), and (c) shown in Figure 5.