How Nematic Torques impact Scalar Active matter: fluctuation-induced renormalization of the persistence length

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We study the impact of nematic torques on scalar active matter and show that they can either promote or suppress phase separation when particles interact via pairwise forces. At the single-particle level, we show that nematic torques enhance particle accumulation at confining boundaries. The underlying mechanism is a fluctuation-induced renormalization of the mass of the polar field due to the nematic torques. This effect quantitatively accounts for all our simulation results and also predicts that nematic torques can suppress demixing in systems comprising active and passive particles.

Model

N particles at positions $\mathbf{r}_i$ and orientations $\hat{u}(\theta_i)$ evolve in 2d according to:

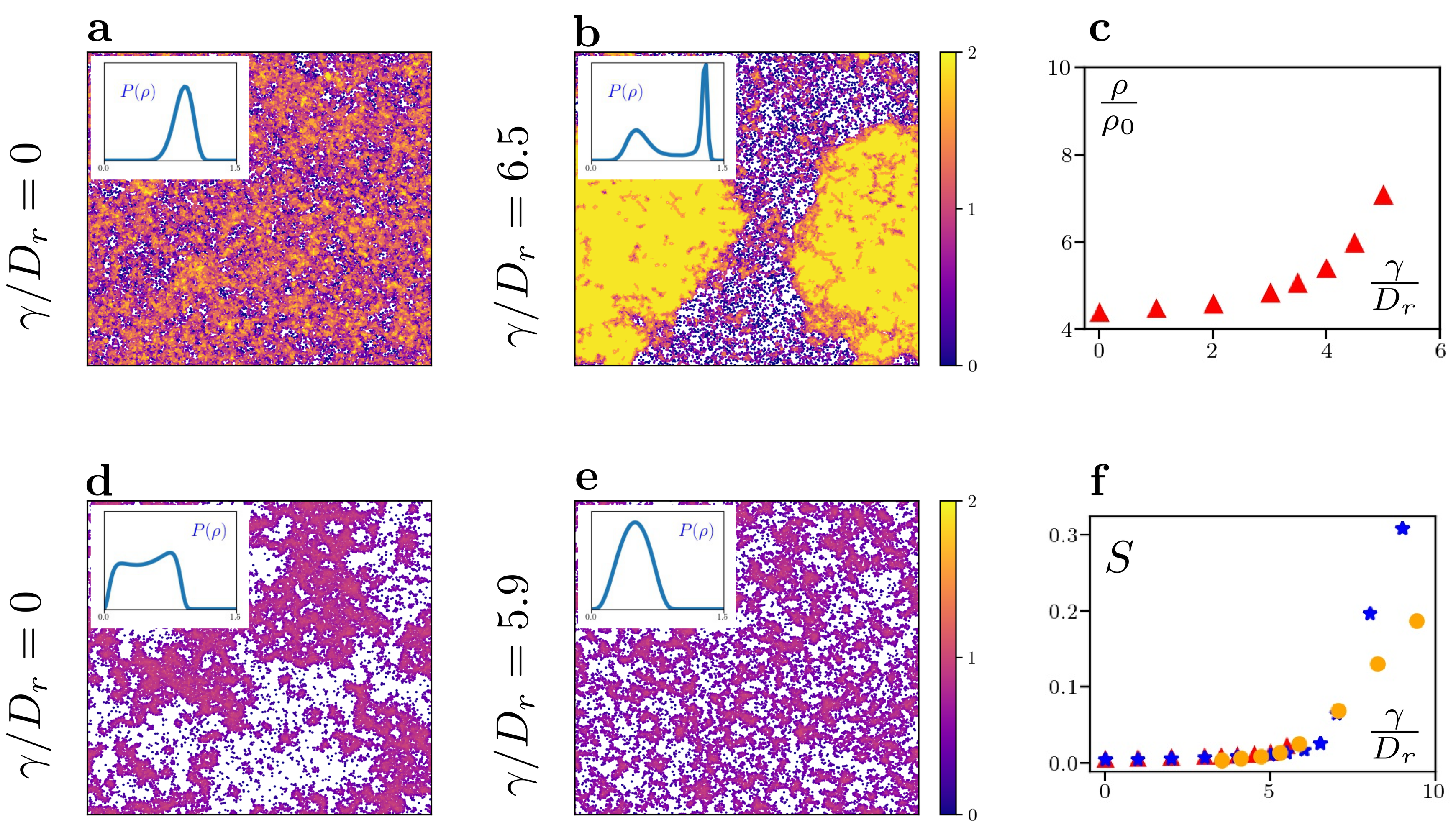
$$\begin{cases} \dot{\mathbf{r}}_i = v_0 \hat{u}(\theta_i) + \mu \sum_{jVi} \mathbf{F}_{ji} + \sqrt{2D_t}\boldsymbol{\eta}_i \\ \dot{\theta}_i = \sqrt{2D_r}\xi_i + \frac{\gamma}{n_i} \sum_{jVi} \sin\left[2(\theta_i - \theta_j)\right] \end{cases} \tag{1}$$

where μ is the particle mobility, $\mathbf{F}_{ji}$ is the force exerted by particle j onto particle i, $\boldsymbol{\eta}_i$ and ξ_i are centered unit-variance Gaussian white noises. Particle i and j interact iff $|\mathbf{r}_i - \mathbf{r}_j| < r_0$ and $n_i = \sum_{jVi} 1$. Finally, D_r and D_t are the rotational and translational diffusivities, respectively.

Phase separation and boundary accumulation

We show below simulations of Eq. (1) with and without nematic torques ($\gamma > 0$ and $\gamma = 0$, respectively), showing that the latter can:

- Promote MIPS in the presence of a WCA potential (**a**→**b**)
- Vaporize the attractive liquid phase for a LJ potential (**d**→**e**)
- Increase the fraction of active particle against a confining boundary (**c**)



All these results are obtained before the global nematic order sets in (**f**).

Renormalization of the persistence time

Using stocastic calculus, we construct the exact dynamics for the empiric measure $\hat{\psi}(\mathbf{r},\theta) \equiv \sum_i \delta(\mathbf{r}-\mathbf{r}_i)\delta(\theta-\theta_i)$. In turn, it yields the evolution for the Fourier modes $\hat{f}_k = \frac{1}{2\pi}\int_0^{2\pi} d\theta \hat{\psi}(\mathbf{r},\theta) e^{ik\theta}$ whose average f_k evolve as

$$\partial_t f_k + \frac{v_0}{2}\left(\nabla^* f_{k+1} + \nabla f_{k-1}\right) + \nabla\cdot\mathbf{I_k} = -k^2 D_r f_k + \left\langle \frac{k\gamma\left(\hat{f}_2 \hat{f}_{k-2} - \hat{f}_{-2}\hat{f}_{k+2}\right)}{2f_0} \right\rangle$$

where $\mathbf{I_k}(\mathbf{r}) \equiv \int d\mathbf{r}' \mathbf{F}(\mathbf{r}-\mathbf{r}') \left\langle \hat{f}_k(\mathbf{r})\hat{f}_0(\mathbf{r}')\right\rangle$ stems from interparticle forces. The first three momenta are $f_0 = \rho$, $f_1 = m_x + i m_y$, $f_2 = q_{xx} + i q_{xy}$, where ρ is the density field, $\mathbf{m}$ is the orientation field, and q_{xx} and q_{xy} are the components of the nematic tensor.
At mean field level the dynamics of f_1 can be shown to read

$$\partial_t f_1 + \frac{v_0}{2}\left(\nabla^* f_2 + \nabla f_0\right) + \nabla \bar{I}_1 = -D_r f_1 + \gamma \frac{f_2}{2f_0} f_1^* - \gamma \frac{f_2^*}{2f_0} f_3$$

In the high temperature phase, $f_2 = 0$ and the persistence time of the orientation field is $1/D_r$. It is thus unaffected by nematic torques [1].

The role of fluctuations can be estimated by considering a simpler system of N fully connected XY spins experiencing the aligning torques of dynamics (1) in the absence of pairwise forces and self-propulsion. There, a perturbative computation shows that the mass of the polar field gets renormalized as

$$D_r \longrightarrow D_r^c(\gamma) \equiv D_r \left(1 + \frac{1}{N}\frac{4\gamma\left(D_r - \gamma\right)}{\left(5D_r - \gamma\right)\left(13D_r - \gamma\right)}\right) \tag{2}$$

The mean-field transition to nematic order happens at $\gamma = 4D_r$. For $D_r < \gamma < 4D_r$, this perturbative computation predicts a decrease of the effective diffusivity $D_r^c(\gamma)$. In turn, this leads to a fluctuation-induced increase of the persistence of active particles in the presence of nematic torques. We checked in homogeneous simulations of Eq. (1) that this increase is indeed observed. To do so, we estimate the mass of the polar field by fitting the auto-correlation of the global orientation $C_M(t) = \langle \mathbf{M}(t+t_0)\cdot\mathbf{M}(t_0)\rangle_{t_0}$ against an exponential, where $\mathbf{M}(t) = \sum_i \mathbf{u}(\theta_i)$. Let us now show how this increased persistence accounts for our numerical results.

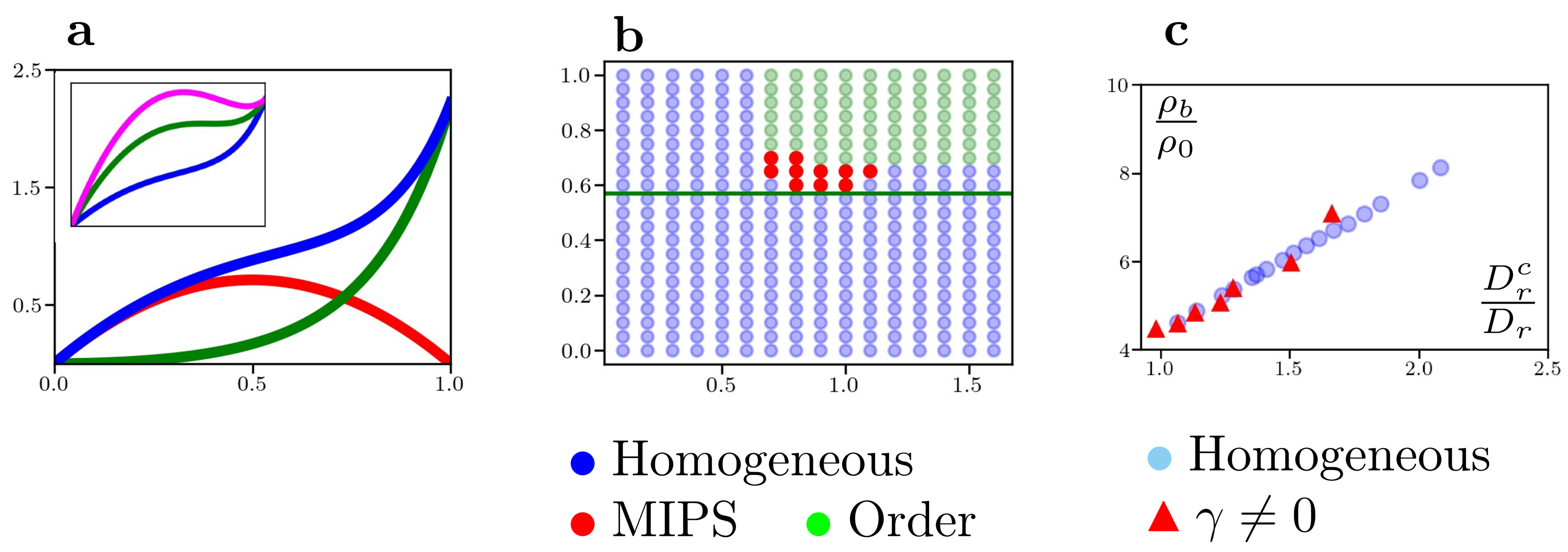
The impact of an enhanced persistence

The dynamics for the density field can be rewritten as $\partial_t \rho = -\mu\nabla\cdot[\nabla\cdot\sigma]$, where σ is a generalized stress tensor given by:

$$\sigma = \sigma^P + \sigma^A$$

$$-\sigma^P_{\alpha\beta} = \frac{D_t}{\mu}\rho\delta_{\alpha\beta} - \sigma^{IK}_{\alpha\beta}, \qquad \sigma^A_{\alpha\beta} = \frac{v_0^2}{2\mu D_r^c(\gamma)}\rho\delta_{\alpha\beta} + \frac{v_0}{\mu D_r^c(\gamma)}\mathrm{I}^{(1)}_{\alpha\beta}$$

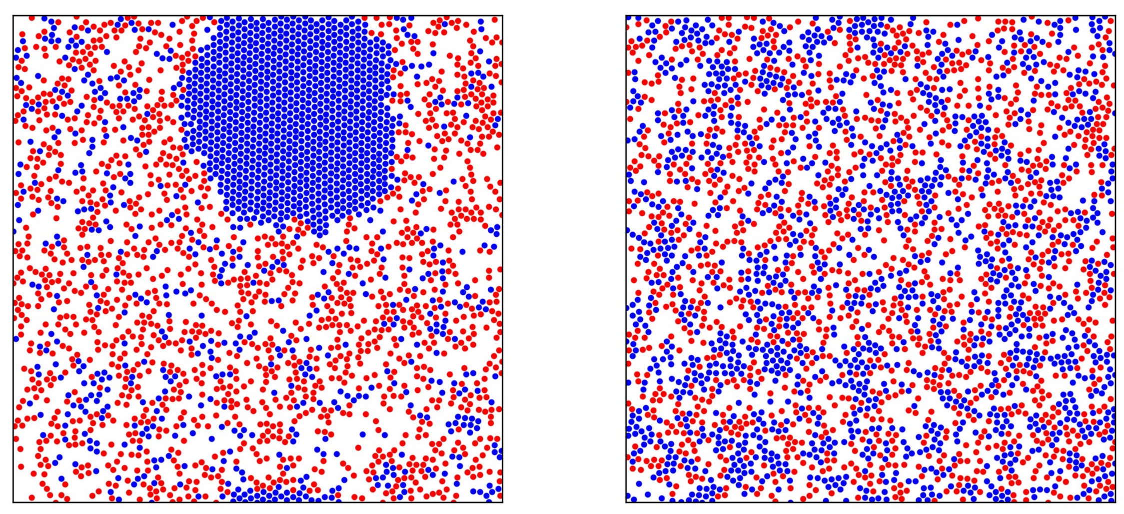
The green part above corresponds to the stress tensor of a passive system of interacting particles. The red part is the active contribution to the stress tensor. Phase separation is expected whenever the generalized compressibility is negative: $-\sigma'(\rho_0) < 0$. Using the measurement of $D_r^c(\gamma)$ in homogeneous systems and scaling argument, we predict a critical alignment strength $\gamma_c \simeq 0.57$, in agreement with numerical simulations (**a-b**).



Finally, the enhanced accumulation at the boundary is quantitatively accounted for by the renormalization of the persistence length (**c**).

Demixing

Using the results of [3], our theory also predicts that nematic torques can suppress demixing in mixtures of active and passive particles by enhancing the persistence of the active component.



References

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