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Supplementary information

Time irreversibility in active matter, from micro to macro

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Supplementary information for Time-irreversibility in active matter, from micro to macro

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1 Entropy production

The forward trajectory $\mathbf{r}(t)$ and $\theta(t)$ uniquely characterize the realization of the noise through

$$\boldsymbol{\eta}(t) = \frac{\dot{\mathbf{r}}(t) - v_0\mathbf{u}(\theta(t))}{\sqrt{2D}} \tag{1}$$

For the reversed trajectory $\mathbf{r}^{\mathrm{r}}(t) = \mathbf{r}(t_f - t)$, $\theta^{\mathrm{r}}(t) = \theta(t_f - t)$ to be observed, the surrounding fluid molecules have to produce a different noise

$$\boldsymbol{\eta}^{\mathrm{r}}(t) = \frac{\dot{\mathbf{r}}^{\mathrm{r}}(t) - v_0\mathbf{u}(\theta^{\mathrm{r}}(t))}{\sqrt{2D}} = \frac{-\dot{\mathbf{r}}(t_f - t) - v_0\mathbf{u}(\theta(t_f - t))}{\sqrt{2D}} = -\boldsymbol{\eta}(t_f - t) - \frac{2v_0\mathbf{u}(\theta(t_f - t))}{\sqrt{2D}} \tag{2}$$

To characterize the irreversibility of the process it is useful to note that the probability of a trajectory is given by its Onsager-Machlup form [1,2]

$$P[\{\mathbf{r}(t), \theta(t)\}] = Z^{-1} P[\{\theta(t)\}|\theta_0] \exp\Big[-\frac{1}{4D}\int_0^{t_f} dt[\dot{\mathbf{r}}(t) - v_0\mathbf{u}(\theta)]^2\Big] P_0(\mathbf{r}_0, \theta_0) \tag{3}$$

where $P[\{\theta(t)\}|\theta_0]$ is the probability of the realization of $\theta(t)$ starting from θ_0, P_0 is the probability of the initial condition, and Z^{-1} is a normalization. Note that, for fully randomizing tumbles, $P[\{\theta(t_f - t)\}|\theta_f] = P[\{\theta(t)\}|\theta_0]$. Taking the logarithm of the ratio between forward and backward trajectories yield the corresponding 'path-wise entropy production' [3] (See also [4,5] for more general results on Markov processes and [6] for discussions of related ideas in the context of dynamical systems):

$$\hat{\Sigma}[\{\mathbf{r}(t), \theta(t)\}] \equiv \log \frac{P[\{\mathbf{r}(t), \theta(t)\}]}{P[\{\mathbf{r}(t_f - t), \theta(t_f - t)\}]} = \frac{\mu}{D}\int_0^{t_f} dt \dot{\mathbf{r}} \cdot \mathbf{f}_p + \log \frac{P_0(\mathbf{r}_0, \theta_0)}{P_f(\mathbf{r}_f, \theta_f)}, \tag{4}$$

where $P_f(\mathbf{r}_f, \theta_f)$ is the probability of being at $\mathbf{r}_f \equiv \mathbf{r}(t_f)$ and $\theta_f \equiv \theta(t_f)$ given that the initial condition was sampled according to P_0.

2 Self-consistency of the effective temperature regime

Let us consider the self-consistency of Eq. (10) of the main text in the presence of a confining potential. Close to the minimum x_0 of the potential, the condition $v_0 \gg \mu V'(x)$ trivially holds. Let us expand the distribution given in Eq. (11) of the main text around x_0. It is then given by a locally Gaussian distribution

$$P(x) \sim \exp\left[-\frac{V''(x_0)(x-x_0)^2}{2T_{\text{eff}}}\right] \tag{5}$$

This predicts a typical displacement $x_t \sim \sqrt{T_{\text{eff}}/V''(x_0)}$ which in turn leads to a typical force that scales as $V'(x_t) \simeq \sqrt{\frac{\tau v_0^2 V''(x_0)}{\mu}}$, where we have used $T_{\text{eff}} = v_0^2\tau/\mu$. The condition $v_0 \gg \mu V'(x)$ then becomes $\mu V''(x_0)\tau \ll 1$: the typical time between two tumbles has to be much shorter than the relaxation time inside the potential well.

3 Non-locality of the steady-state distribution

Consider the effective potential given in Eq. (11) in the main text. Its non-local nature becomes apparent if one adds a localized perturbation $\delta V(x) = \epsilon\delta(x-y)$, centered around y, to the potential $V(x)$. The effective potential $V_{\text{eff}}(x)$ then picks up a contribution due to δV, because of the term $\frac{\int^x V'(y)^2 V^{(3)}(y)dy}{2}$. To linear order in ϵ, it reads

$$\delta V_{\text{eff}}(x) = \frac{\epsilon\tau^2}{2}[(V'(y)^2)^{(3)} + 2V''(y)V^{(3)}(y) + 2V'(y)V^{(4)}(y)]\Theta(x-y)\ , \tag{6}$$

which adds a global step to the density profile at $x = y$.

4 Self-propelled ABPs interacting via a Lennard-Jones potential

We consider N active Brownian particles evolving in two space dimensions under the dynamics:

$$\dot{\mathbf{r}}_i = v_0\mathbf{u}(\theta_i) - \sum_j \nabla V(\mathbf{r}_i - \mathbf{r}_j) + \sqrt{2D_t}\boldsymbol{\eta}_i \qquad \dot{\theta}_i = \sqrt{2D_r}\xi_i \tag{7}$$

where $\boldsymbol{\eta}_i$ and ξ_i are independant Gaussian white noises, and V is the Lennard-Jones potential

$$V(\mathbf{r}) = 4\varepsilon\left(\frac{\sigma^{12}}{\mathbf{r}^{12}} - \frac{\sigma^6}{\mathbf{r}^6}\right)\ . \tag{8}$$

Interactions between particles are truncated at $|\mathbf{r}| = 2.7\sigma$ and we used periodic boundary conditions. Figure 5a in the main text was obtained using $\sigma = 0.37$, $T = 0.4$ and $D_r = 2$. The

phase-separated regions were found by running simulations for $\rho_0 = 2.5\sigma^2$ ($v_0 < 8$) and $\rho_0 = 4\sigma^2$ ($v_0 > 8$) in systems of line sizes $L = 80$ up to $t = 2\,000$, where ρ_0 is the rescaled number density $\rho_0 \equiv N\sigma^2/L^2$. The symbols correspond to estimates of the coexisting densities. The latter were obtained from the local maxima of histograms of the density field, constructed using bins of linear size 4.

1. Onsager, L. & Machlup, S. Fluctuations and irreversible processes. *Physical Review* **91**, 1505 (1953).

2. Woillez, E., Zhao, Y., Kafri, Y., Lecomte, V. & Tailleur, J. Activated escape of a self-propelled particle from a metastable state. *Phys. Rev. Lett.* **122**, 258001 (2019). URL `https://link.aps.org/doi/10.1103/PhysRevLett.122.258001`.

3. Seifert, U. Entropy production along a stochastic trajectory and an integral fluctuation theorem. *Physical review letters* **95**, 040602 (2005).

4. Maes, C. The fluctuation theorem as a gibbs property. *Journal of statistical physics* **95**, 367–392 (1999).

5. Maes, C., Redig, F. & Moffaert, A. V. On the definition of entropy production, via examples. *Journal of mathematical physics* **41**, 1528–1554 (2000).

6. Gaspard, P. *Chaos, Scattering and Statistical Mechanics*. Cambridge Nonlinear Science Series (Cambridge University Press, 1998).