Supplemental material: Thermodynamic cycles with active matter

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SIMULATION DETAILS

To produce numerical results, we evolved the stochastic differential equations describing Active Brownian Particles (ABPs) using an Euler stepping algorithm in C for both the translational (x, y) and orientational (θ) degrees of freedom, which we will collectively denote by \mathbf{Q} . We discretize the simulation time in units of Δt (at most 10^{-4}) and the simulation time is then $t_i = i\Delta t$ for integer i. The coordinates at the start of the time t_i are denoted $\mathbf{Q}(t_i) \equiv \mathbf{Q}_i$

$$x_{i+1} = x_i + F(x_i, \theta_i) \Delta t + \sqrt{2D_t \Delta t} \, \tilde{\eta}_x,$$

$$y_{i+1} = y_i + v \sin \theta \Delta t + \sqrt{2D_t \Delta t} \, \tilde{\eta}_y,$$

$$\theta_{i+1} = \theta_i + \mu_r \Gamma(\theta_i, x_i) \Delta t + \sqrt{2D_r \Delta t} \, \tilde{\eta}_\theta,$$
(1)

with $F(x,\theta) = v \cos \theta - \lambda \mu_t \left[(x-\ell)H(x-\ell) + xH(-x) \right]$ and $\Gamma(\theta,x) = \lambda \kappa \sin(2\theta) \left[H(x-\ell) + H(-x) \right]$. All the $\tilde{\eta}_Q$ are zero-mean unit-variance Gaussian random variables, and we set $\mu_r = \mu_t = 1$ in the simulations.

The calculation of observables that are a function of (x,y,θ) is straightforward. Note that we can write the number density as

$$P(\mathbf{Q}_i) = \sum_{k=1}^{N} \delta(\mathbf{Q}_i^k - \mathbf{Q}_i)$$

$$= \sum_{k=1}^{N} \delta(x_i^k - x)\delta(y_i^k - y)\delta(\theta_i^k - \theta).$$
(2)

For a given observable $\mathcal{O}(x(t_i), y(t_i), \theta(t_i))$, the ensemble average is numerically calculated as

$$\langle \mathcal{O}(x(t_i), y(t_i), \theta(t_i)) \rangle = \sum_{k=1}^{N} \mathcal{O}(x_i^k, y_i^k, \theta_i^k).$$
 (3)

At the start of the simulation, all the particles are randomly distributed within the domain and are left to undergo the stochastic dynamics described by (1) for some initialization time, at least $10^6 \Delta t$. The cycle is then implemented by incrementing the control parameters deterministically as

$$\lambda_{i+1} = \lambda_i + \Delta \lambda, \quad \ell_{i+1} = \ell_i + \Delta \ell.$$
 (4)

For quasistatic calculations, the cycles under investigation are split into many smaller segments. Observables such as work are calculated separately within each segment and then summed to gain the total work output. The steps in (ℓ, λ) are sufficiently small to assure

effective steady state profiles at each stage of the cycle. The color scaling in Fig. 2(b) of the main text follows ($|\mathcal{W}_{qs}|/\mathcal{W}_{qs}$) $\ln(1+|\mathcal{W}_{qs}|)$. For finite-time cycles, we run the full cycle and collect averages for the extracted work output and dissipated heat. The work output as a function of cycle time is found to obey the form $\mathcal{W} = \mathcal{W}_{QS}(1-\tau_r/\tau_c)$, with the dimensionless fitting parameter $\tau_r D_r = (2.9 \pm 0.4) \times 10^4$ for Fig. 3 in the main text. We report the parameter values for Figs. 2-3 of the main text in Tab. I.

DEPLETION OF BULK DENSITY

In this Section, we calculate the bulk density which is depleted from the hard wall density N/ℓ due to the penetration of particles into the boundary. The precise form is derived in this Section on approximating the position distribution m_0 by a Boltzmann factor as $m_0(x) = \rho(\ell, \lambda) \exp\left[-\mu_t u_t(x)/(D_t(1+\text{Pe}))\right]$, where the bulk density $\rho(\ell, \lambda)$ depends both on ℓ and λ . For harmonic confinement, we get

$$N = \int_{-\infty}^{+\infty} m_0(x) dx$$

$$= \rho(\ell, \lambda) \left\{ \ell + 2 \int_{\ell}^{\infty} \exp\left[-\frac{\mu_t \lambda (x - \ell)^2}{2D_t (1 + \text{Pe})} \right] dx \right\}$$
(5)
$$= \rho(\ell, \lambda) \left[\ell + \sqrt{\frac{2\pi D_t (1 + \text{Pe})}{\mu_t \lambda}} \right],$$

where we have used the reflection symmetry with respect to the centre of the box, yielding

$$\rho(\ell,\lambda) = \frac{N}{\ell + \sqrt{2\pi D_{t}(1 + \text{Pe})/(\lambda \mu_{t})}}.$$
 (6)

The number of particles within one wall follows as

$$\int_{\ell}^{\infty} m_0 dx = N - \ell \, \rho(\ell, \lambda). \tag{7}$$

ANGULAR MOMENTS OF THE FOKKER-PLANCK DISTRIBUTION

In this Section, we outline the derivation of the hierarchy of equation for the angular moments defined as

$$m_n(x) = \int_0^{2\pi} \cos(n\theta) \mathcal{P}(x,\theta) d\theta, \tag{8}$$

 $D_{\rm t}$ N $D_{\rm r}$ ℓ_i , ℓ_f $\lambda_{
m i},\,\lambda_{
m f}$ L_y κ $\mu_{\rm t}, \mu_{\rm r}$ 20 6.32 - , -0.2100 Fig. 2(a) 1 1, 1 - , -6000 Fig. 2(b) 1 1, 1 20 20, 40 6, 10 6000 100 Figs. 2(c-e) 5, 15, 30 6.32 1, 1 100 40, 50 0.3, 0.5100 6000Fig. 3 6.32 1.1 20 20, 40 0.3, 0.540 100 6000

TABLE I. Simulation/Plotting parameters for data in Figs. 2-3 of the main text.

where $\mathcal{P}(x,\theta)$ is the stationary probability density of position x and angle θ . Alternatively, $\mathcal{P}(x,\theta)$ can be written as an even Fourier series:

$$\mathcal{P}(x,\theta) = \frac{1}{2\pi} m_0(x) + \frac{1}{\pi} \sum_{n=1}^{\infty} m_n(x) \cos(n\theta), \quad (9)$$

since the $\sin(n\theta)$ terms, that are odd in angle, have vanishing coefficients by symmetry. Within the wall regions, namely for x < 0 and $x > \ell$, the full steady-state Fokker-Planck equation for ABPs with harmonic wall confinement is

$$0 = -\partial_x \left[\left(v \cos \theta - \mu_t \partial_x u_t \right) \mathcal{P} - D_t \partial_x \mathcal{P} \right] - \partial_\theta \left[\lambda \kappa \mu_T \sin(2\theta) \mathcal{P} - D_T \partial_\theta \mathcal{P} \right].$$
 (10)

Substituting (9) into (10) and collecting the coefficients of $cos(n\theta)$ gives the hierarchy of moment equations

$$n^{2}D_{r}m_{n} + \frac{\lambda \kappa \mu_{r}n}{2}(m_{n-2} - m_{n+2})$$

$$= -\partial_{x}\left(v\frac{m_{n+1} + m_{n-1}}{2} - \mu_{t}m_{n}\partial_{x}u_{t} - D_{t}\partial_{x}m_{n}\right). \tag{11}$$

Evaluating the $n^{\rm th}$ moment requires deriving all the moments up to $n \pm 2$. Of particular note is the n = 0 condition, which reads

$$\partial_x (v m_1 - \mu_t m_0 \partial_x u_t - D_t \partial_x m_0) = 0, \tag{12}$$

where we have used that $m_n = m_{-n}$ which follows from the definition of the moments. This is a statement of conserved particle flux. For a confined system, the flux is zero everywhere, which manifests as

$$vm_1 - \mu_t m_0 \partial_x u_t - D_t \partial_x m_0 = 0. \tag{13}$$

Furthermore, it is useful to note for the following Sections that all angular moments have definite parity about the centre of the box. Indeed, using $\mathcal{P}(x,\theta) = \mathcal{P}(\ell-x,\pi-\theta)$ we get

$$\int_{0}^{2\pi} \cos(n\theta) \mathcal{P}(x,\theta) d\theta$$

$$= \int_{0}^{2\pi} \cos(n\theta) \mathcal{P}(\ell - x, \pi - \theta) d\theta$$

$$= \int_{\pi}^{-\pi} \cos[n(\phi - \pi)] \mathcal{P}(\ell - x, \phi) d\phi$$

$$= (-1)^{n} \int_{-\pi}^{\pi} \cos(n\phi) \mathcal{P}(\ell - x, \phi) d\phi.$$
(14)

In the language of moments, this says that

$$m_n(x) = (-1)^n m_n(\ell - x).$$
 (15)

All moments are odd or even in space depending on their order. This shows that only the even angular moments are non-zero when integrated over all space, since the odd ones must vanish by symmetry.

To compute explicitly the expression of angular moments integrated over the wall regions, we introduce angular functions $f_{\pm}(\theta)$ by integrating \mathcal{P} in (9) over the right wall $(x:\ell\to\infty)$ and the left wall $(x:-\infty\to 0)$, respectively, yielding

$$f_{\pm}(\theta) = \frac{1}{2\pi} \int_{\ell}^{\infty} m_0 dx$$
$$+ \frac{1}{\pi} \sum_{n=1}^{\infty} (\pm 1)^n \cos(n\theta) \int_{\ell}^{\infty} m_n dx.$$
(16)

Note that for $f_{-}(\theta)$ we have used (15) to redefine the integration range. We then integrate the Fokker-Plank equation (10) to the right and left of the box in the same way, yielding two differential equations:

$$0 = v \cos \theta \, \mathcal{P}(\ell, \theta) + D_{\rm r} \partial_{\theta}^{2} f_{+} - \mu_{\rm r} \partial_{\theta} (\Gamma f_{+}),$$

$$0 = -v \cos \theta \, \mathcal{P}(0, \theta) + D_{\rm r} \partial_{\theta}^{2} f_{-} - \mu_{\rm r} \partial_{\theta} (\Gamma f_{-}).$$
(17)

Next, we define the symmetric/antisymmetric linear combinations $F_{\pm} = (f_{-} \pm f_{+})/2$, which satisfy the equations

$$0 = \frac{1}{2}v\cos\theta \left[\mathcal{P}(\ell,\theta) \mp \mathcal{P}(0,\theta) \right] + D_{\rm r}\partial_{\theta}^{2}F_{\pm} - \mu_{\rm r}\partial_{\theta}(\Gamma F_{\pm}).$$
(18)

To provide an explicit solution for F_{\pm} , we assume that the distribution is flat everywhere outside of the wall region, so that $\mathcal{P}(x,\theta) = \rho(\ell,\lambda)/(2\pi)$ within the bulk, which formally neglects any effects due to boundary accumulation provided that the rotational diffusion coefficient is large enough $(D_{\rm r} \gg \lambda \mu_{\rm t})$. The equations for F_{\pm} then simplify to

$$0 = D_{\rm r} \partial_{\theta} F_{+} - \mu_{\rm r} \Gamma F_{+},$$

$$0 = \frac{v \rho(\ell, \lambda)}{2\pi} \sin \theta + D_{\rm r} \partial_{\theta} F_{-} - \mu_{\rm r} \Gamma F_{-},$$
(19)

yielding

$$F_{+} = A \exp\left[\frac{\mu_{\rm r}}{D_{\rm r}} \int^{\theta} \Gamma(\theta') d\theta'\right] = A \exp\left[-\frac{\lambda_{\kappa}}{2} \cos(2\theta)\right], \tag{20}$$

where A is determined through normalisation. From (15-16), we get

$$\int_0^{2\pi} F_+(\theta) d\theta = \frac{1}{2} \left[\int_{\ell}^{\infty} m_0 dx + \int_{-\infty}^0 m_0 dx \right]$$
$$= \int_{\ell}^{\infty} m_0 dx.$$
(21)

Using this condition, we derive the full solution for F_+ :

$$F_{+}(\theta) = \frac{2 \exp(-\lambda_{\kappa} \cos(2\theta)/2)}{\pi I_{0}(\lambda_{\kappa}/2)} \int_{\ell}^{\infty} m_{0} dx, \qquad (22)$$

where $I_n(x)$ is the modified Bessel function of the first kind. The integral over even angular moments then come from calculating the Fourier coefficients of F_+ :

$$\int_{\ell}^{\infty} m_{2n} dx = \int_{0}^{2\pi} F_{+}(\theta) \cos(2n\theta) d\theta$$
$$= (-1)^{n} \frac{I_{n}(\lambda_{\kappa}/2)}{I_{0}(\lambda_{\kappa}/2)} \int_{\ell}^{\infty} m_{0} dx.$$
 (23)

Similarly, the expression for F_{-} follows by solving (19):

$$F_{-}(\theta) = -\frac{v\rho(\ell,\lambda)}{2D_{\rm r}} \sqrt{\frac{\pi}{\lambda_{\kappa}}} e^{-\lambda_{\kappa}[1+\cos(2\theta)]/2} \operatorname{erfi}\left[\sqrt{\lambda_{\kappa}}\cos\theta\right],$$
(24)

where we have used the boundary condition $F_{-}(\pi/2) = 0$ deduced from (15-16), and the "imaginary error function" is defined by

$$\operatorname{erfi}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{y^2} dy. \tag{25}$$

The integral over odd angular moments is then given by

$$\int_{\ell}^{\infty} m_{2n+1} dx = \int_{0}^{2\pi} F_{-}(\theta) \cos[(2n+1)\theta] d\theta$$

$$= -\frac{v\rho(\ell,\lambda)}{D_{r}} \sqrt{\frac{\pi}{\lambda_{\kappa}}} \int_{0}^{\pi} \cos[(2n+1)\theta]$$

$$\times e^{-\lambda_{\kappa}(1+\cos(2\theta)]/2} \operatorname{erfi}\left[\sqrt{\lambda_{\kappa}} \cos\theta\right] d\theta.$$
(26)

At n=0, this integral can be done exactly to obtain the function ϕ defined in (5) of the main text, and which has been calculated in prior work by Solon *et al.* (Ref. [30] in main text) through a different method.

AVERAGE POTENTIAL ENERGIES

In this Section, we derive the expression for ψ and χ which appear in the average confining and aligning potential energies, see (7) of main text. To this end, we calculate the energy in the right hand wall only, and then obtain the energy for the entire system by doubling the answer. It is convenient for the following calculations to

define two dimensionless parameters, both of which are scaled wall stiffnesses:

$$\lambda_t = \lambda \mu_t / D_r, \quad \lambda_\kappa = \lambda \mu_r \kappa / D_r.$$
 (27)

Denoting the confining potential energy in the right hand wall as $\langle u_{\rm t} \rangle_r$, we can write that

$$\langle u_{\rm t} \rangle_r = \int_{\ell}^{\infty} m_0(x) u_{\rm t}(x) \mathrm{d}x,$$
 (28)

and, for a harmonic potential $u_t \propto (x - \ell)^2$, we get

$$\langle u_{\rm t} \rangle_r = \int_{\ell}^{\infty} m_0 \frac{x - \ell}{2} \partial_x u_{\rm t} \mathrm{d}x.$$
 (29)

Using (13), we then deduce

$$\langle u_{t} \rangle_{r} = \frac{1}{\mu_{t}} \int_{\ell}^{\infty} \left(v m_{1} - D_{t} \partial_{x} m_{0} \right) \frac{x - \ell}{2} dx$$

$$= \frac{v}{2\mu_{t} \lambda} \int_{\ell}^{\infty} m_{1} \partial_{x} u_{t} dx - \frac{D_{t}}{2\mu_{t} \lambda} \int_{\ell}^{\infty} (\partial_{x} m_{0}) \partial_{x} u_{t} dx,$$
(30)

and after integrating the last term by parts we get

$$\langle u_{\rm t} \rangle_r = \frac{v}{2\mu_{\rm t}\lambda} \int_{\ell}^{\infty} m_1 \partial_x u_{\rm t} dx + \frac{D_{\rm t}}{2\mu_{\rm t}} \int_{\ell}^{\infty} m_0 dx.$$
 (31)

Thus, we need to evaluate the integral $\int m_1 \partial_x u_t dx$.

To this end, we introduce the angular functions $g_{\pm}(\theta)$ defined by

$$g_{\pm}(\theta) = \pm \frac{1}{2\pi} \int_{\ell}^{\infty} m_0 \partial_x u_t dx + \frac{1}{\pi} \sum_{n=1}^{\infty} (\pm 1)^{n+1} \cos(n\theta) \int_{\ell}^{\infty} m_n \partial_x u_t dx.$$
(32)

We multiply (10) by $\partial_x u_t$ and integrate over x to get

$$D_{\rm r}\partial_{\theta}^{2}g_{\pm} - \mu_{\rm r}\partial_{\theta}(\Gamma g_{\pm}) + \lambda v \cos\theta f_{\pm} - \lambda \mu_{\rm t}g_{\pm} = \mp \lambda D_{\rm t}\mathcal{P}(0,\theta),$$
(33)
where f_{\pm} is defined in (16). We define $G_{+} = (g_{+} + g_{-})/2$,

$$G_{+}(\theta) = \frac{1}{\pi} \sum_{n=0}^{\infty} \cos[(2n+1)\theta] \int_{\ell}^{\infty} m_{2n+1} \partial_x u_{t} dx. \quad (34)$$

Therefore, evaluating G_+ and taking its first Fourier coefficient allows one to evaluate $\int m_1 \partial_x u_t dx$:

$$\int_{\ell}^{\infty} m_1 \partial_x u_t dx = \int_{0}^{2\pi} G_+(\theta) \cos \theta d\theta.$$
 (35)

From (33), we deduce that G_+ satisfies the equation:

$$D_{\mathbf{r}}\partial_{\theta}^{2}G_{+} - \mu_{\mathbf{r}}\partial_{\theta}(\Gamma G_{+}) - \lambda\mu_{\mathbf{t}}G_{+} = -\lambda v\cos\theta F_{+}. \quad (36)$$

The solution can be written implicitly in terms of the Green's function \mathcal{G} satisfying

$$\partial_{\theta}^{2} \mathcal{G} - \lambda_{\kappa} \partial_{\theta} \left[\sin(2\theta) \mathcal{G} \right] = \delta(\theta - \zeta), \tag{37}$$

so that

$$G_{+}(\eta_{1}) = \lambda_{t} \int_{0}^{2\pi} \mathcal{G}(\eta_{1}, \eta_{2}) \left[G_{+}(\eta_{2}) - \frac{v \cos \eta_{2}}{\mu_{t}} F_{+}(\eta_{2}) \right] d\eta_{2}.$$
(38)

When considering the first Fourier component of G_+ as in (35), we get

$$\int_{\ell}^{\infty} m_1 \partial_x u_t dx = \lambda_t \int_{0}^{2\pi} \cos \eta_1 \mathcal{G}(\eta_1, \eta_2) d\eta_1 d\eta_2$$

$$\times \left[G_+(\eta_2) - \frac{v \cos \eta_2}{\mu_t} F_+(\eta_2) \right].$$
(39)

To proceed further, we assume that the Green's function \mathcal{G} can be written as

$$G(\eta_1, \eta_2) = \frac{1}{\pi} \sum_{m=1}^{\infty} \tilde{G}_m \cos[m(\eta_1 - \eta_2)],$$
 (40)

with constant coefficients $\tilde{\mathcal{G}}_m$. This is not true generically since (37) is not translationally invariant with respect to θ . Hence, we expect the approximate form (40) to hold for small $\lambda \mu_r \kappa/D_r$, as this parameter controls the strength of the term breaking translational invariance in (37). Substituting (40) in (39), we integrate over angles to get

$$\int_{\ell}^{\infty} m_1 \partial_x u_t dx = \lambda_t \tilde{\mathcal{G}}_1 \int d\eta \cos \eta G_+(\eta) - \frac{v}{\mu_t} \lambda_t \tilde{\mathcal{G}}_1 \int_0^{2\pi} \cos^2(\eta) F_+(\eta) d\eta.$$
(41)

Noting that the first integral on the right hand side is again the first Fourier coefficient of G_+ , we obtain

$$\int_{\ell}^{\infty} m_{1} \partial_{x} u_{t} dx$$

$$= \frac{v}{\mu_{t}} \frac{\lambda_{t} \tilde{\mathcal{G}}_{1}(\lambda_{\kappa})}{\lambda_{t} \tilde{\mathcal{G}}_{1}(\lambda_{\kappa}) - 1} \int_{0}^{2\pi} \cos^{2}(\eta) F_{+}(\eta) d\eta$$

$$= \frac{v}{2\mu_{t}} \frac{\lambda_{t} \tilde{\mathcal{G}}_{1}(\lambda_{\kappa}) - 1}{\lambda_{t} \tilde{\mathcal{G}}_{1}(\lambda_{\kappa}) - 1} \left[1 - \frac{I_{1}(\lambda_{\kappa}/2)}{I_{0}(\lambda_{\kappa}/2)} \right] \int_{\ell}^{\infty} m_{0} dx,$$
(42)

where we have used (22). It now remains to evaluate $\tilde{\mathcal{G}}_1$. In what follows, we show that $\tilde{\mathcal{G}}_1 = -\phi(\lambda_{\kappa})$ where the function $\phi(z) = (1 - e^{-z})/z$ appears in (5) of the main text. The mechanical pressure P is defined as

$$P = \int_{\ell}^{\infty} m_0 \partial_x u_t dx$$

$$= \frac{v}{\mu_t} \int_{\ell}^{\infty} m_1 dx + \frac{D_t}{\mu_t} \rho(\ell, \lambda),$$
(43)

where we have used (13). Comparing (43) with (5) of the main text, we deduce

$$\int_{\ell}^{\infty} m_1 dx = \frac{v\rho(\ell, \lambda)}{2D_r} \phi(\lambda_{\kappa}). \tag{44}$$

The function F_{-} satisfies the differential equation (19) whose solution can be written in terms of \mathcal{G} as

$$F_{-}(\theta) = -\frac{v\rho(\ell,\lambda)}{2\pi D_{\rm r}} \int_{0}^{2\pi} \mathcal{G}(\theta,\eta) \cos\eta \,\mathrm{d}\eta. \tag{45}$$

Taking the first Fourier coefficient of F_{-} then provides access to $\int m_1(x) dx$ as

$$\int_{\ell}^{\infty} m_{1}(x) dx = \int_{0}^{2\pi} F_{-}(\theta) \cos \theta d\theta$$

$$= -\frac{v\rho(\ell, \lambda)}{2\pi D_{r}} \iint \mathcal{G}(\theta, \eta) \cos \theta \cos \eta d\theta d\eta$$

$$= -\frac{v\rho(\ell, \lambda)}{2D_{r}} \tilde{\mathcal{G}}_{1},$$
(46)

from which $\tilde{\mathcal{G}} = -\phi(\lambda_{\kappa})$ follows using (44). Then, using (31) and (42), the average confining potential energy reads

$$\langle u_{\rm t} \rangle = \frac{D_{\rm t}}{\mu_{\rm t}} (1 + \text{Pe}\,\psi) \int_{\ell}^{\infty} m_0 dx,$$

$$\psi = \frac{\phi(\lambda_{\kappa})}{1 + \lambda_t \,\phi(\lambda_{\kappa})} \left[1 - \frac{I_1(\lambda_{\kappa}/2)}{I_0(\lambda_{\kappa}/2)} \right],$$
(47)

as presented in (7) of the main text.

Finally, the average aligning potential energy is defined as

$$\langle u_{\rm r} \rangle = \frac{\lambda \kappa}{2} \langle \cos(2\theta) [H(-x) + H(x-\ell)] \rangle,$$
 (48)

which follows directly from (23) as

$$\langle u_{\rm r} \rangle = -\frac{\lambda \kappa \chi}{2} \int_{\ell}^{\infty} m_0 dx, \quad \chi = \frac{I_1(\lambda_{\kappa}/2)}{I_0(\lambda_{\kappa}/2)},$$
 (49)

as presented in (7) of the main text.