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Pressure is not a state function for generic active fluids

I. DETAILS OF NUMERICAL SIMULATIONS

Time-stepping: Simulations were run using Euler time-discretization schemes over total times $T = 10^4$ or larger (up to $T = 10^9$).

Non-interacting particles: At each time step dt, particles update their direction of motion θ_i, then their position $\mathbf{r_i}$. For ABPs, $\dot{\theta}_i = \sqrt{2D_r}\xi(t)$ where $\xi(t)$ is a Gaussian white noise of unit variance. For RTPs, the time Δt before the next tumble is chosen using an exponential distribution $P(\Delta t) = \lambda e^{-\lambda \Delta t}$. When this time is reached, a new direction is chosen uniformly in $[0, 2\pi[$ and the next tumble time is drawn from the same distribution. This neglects the possibility to have two tumbles during dt. Both types of particles then move according to the Langevin equation $\dot{\mathbf{r_i}} = v\mathbf{e}_{\theta_\mathbf{i}} - \nabla V + \sqrt{2D_t}\eta(t)$ where $\eta(t)$ is a Gaussian white noise of unit variance.

Hard-core repulsion: To model hard-core repulsion we use a WCA potential $V(r) = 4\big[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\big] + 1$ if $r < 2^{1/6}\sigma$ and 0 otherwise. The unit of length is chosen such that the interaction radius $2^{1/6}\sigma = 1$. Because of the stiff repulsion, one needs to use much smaller time steps ($dt = 5.10^{-5}$ for the speeds considered in the paper).

Aligning particles: Particles exert torques on each other to align their directions of motion θ_i. The torque exerted by particle j on particle i reads $F(\theta_j - \theta_i, \mathbf{r}_j - \mathbf{r}_i) = \frac{\gamma}{\mathcal{N}(\mathbf{r}_i)}\sin(\theta_j - \theta_i)$ if $|\mathbf{r}_i - \mathbf{r}_j| < R$ and 0 otherwise, where $\mathcal{N}(\mathbf{r}_i)$ is the number of particles interacting with particle i. The interaction radius R is chosen as unit of length. For the parameters used in simulations $v = 1$, $\gamma = 2$, with a time-step $dt = 10^{-2}$.

Quorum sensing $v(\bar{\rho})$: The velocities of the particles depend on the local density $\bar{\rho}$. The unit of length is fixed such that the radius of interaction is 1. To compute the local density, we use the Schwartz bell curve $K(r) = \frac{1}{Z}\exp(-\frac{1}{1-r^2})$ for $r < 1$ and 0 otherwise, where Z is a normalization constant. The average density around particle i is then given by $\bar{\rho}_i = \sum_j K(|\mathbf{r_i} - \mathbf{r_j}|)$ and the velocity of particle i is $v(\bar{\rho}_i) = v_0(1 - \bar{\rho}_i/\rho_m) + v_1$. We used $dt = 5.10^{-3}$.

Asymmetric wall experiment: The simulation box is separated in two parts by an asymmetric wall which has a different stiffness λ_1 and λ_2 on both sides. At each time step, the total force $\mathcal{F}$ exerted on the wall by the particles is computed and the wall position is updated according to $\dot{x}_{\rm wall} = \mu_{\rm wall}\mathcal{F}$, where $\mu_{\rm wall} = 2.\,10^{-4} \ll \mu_t$ is the wall mobility.

SI movie 1: Asymmetric wall experiment with non-interacting ABP particles. The particles are spherical (no torque) for $t < 1000$ and $t > 3000$ and ellipses with $\kappa = 1$ for $1000 < t < 3000$. Wall potentials are harmonic and other parameters are $v = 10$, $D_r = 1$, $\lambda = 10$ (external box) and for the asymmetric mobile wall $\lambda = 1$ on the left and $\lambda = 4$ on the right.

II. EQUILIBRIUM PRESSURE

Here, for completeness, we show that in equilibrium 1) the thermodynamic pressure equals the mechanical pressure given by Eq. (3) of the main text, and 2) that it is independent from the wall potential. For simplicity we consider a system of interacting point-like particles in one-dimension where the pressure is a force and we work in the canonical ensemble. The extension to other cases

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is trivial.

The thermodynamic pressure is defined as

$$P = -\left.\frac{\partial F}{\partial L}\right|_N \ , \tag{1}$$

where L is the system length, F is the free energy, and the number of particles N is kept constant. Note that since F is extensive, any contribution from the potential of the wall is finite and will therefore not influence the pressure. Next, the free energy is given by

$$F = -\frac{1}{\beta}\ln \mathcal{Z} \ , \tag{2}$$

where

$$\mathcal{Z} = \sum_n e^{-\beta[(\mathcal{H}+\sum_i V(x_i-L)]} \ , \tag{3}$$

is the partition function, $\beta = 1/T$ with T the temperature, and the sum runs over all micro-states. The origin of the wall is chosen at $x = L$, as opposed to $x = x_w$ in the main text. The energy function of the system is given by $\mathcal{H}+\sum_i V(x_i-L)$, where $V(x_i-L)$ is the wall potential, x_i is the position of particle i, and $\mathcal{H}$ contains all the other interactions in the system. Using the definition of P we have

$$P = -\frac{1}{\mathcal{Z}}\sum_n\sum_i \partial_L V(x_i-L)e^{-\beta(\mathcal{H}+\sum_i V(x_i-L))} = -\left\langle \int dx\rho(x)\partial_L V(x-L)\right\rangle \ , \tag{4}$$

where the angular brackets denote a thermal average, and $\rho(x) = \sum_i \delta(x-x_i)$ is the number density. Exchanging ∂_L for $-\partial_x$, we obtain the expression from the main text

$$P = \left\langle \int dx\rho(x)\partial_x V(x-L)\right\rangle \ . \tag{5}$$

III. DERIVATION OF THE PRESSURE FOR NON-INTERACTING SPPS

To compute the mechanical pressure P for SPPs, we first define $m_n(x) = \int_0^{2\pi}\cos(n\theta)\mathcal{P}(x,\theta)d\theta$. Taking moments of the master equation, Eq. (2) in the main text, we find that in steady state

$$0 = -\partial_x(vm_1 - \mu_t\rho\partial_x V - D_t\partial_x\rho) \ , \tag{6}$$

$$(D_r+\alpha)m_1 = -\partial_x\Big(v\frac{\rho+m_2}{2} - \mu_t m_1\partial_x V - D_t\partial_x m_1\Big) - \int_0^{2\pi}\sin\theta\,\mu_r\Gamma(x,\theta)\mathcal{P}\,d\theta \ . \tag{7}$$

Equation (6) is tantamount to setting $\partial_x J = 0$, where J is a particle current that must vanish in any confined system; while Eq. (7) expresses a similar result for the first moment m_1. Equation (3) of the main text and Eq. (6) together imply that

$$P = \int_0^\infty \frac{1}{\mu_t}\left[vm_1 - D_t\partial_x\rho\right]\,dx \ . \tag{8}$$

Next, from Eqs. (6,7) we see that, apart from the term involving the torque Γ, $m_1(x)$ is a total derivative. We can trivially integrate this contribution to Eq. (8), noting that at $x = 0$, isotropic bulk conditions prevail so that $m_1 = m_2 = 0$, and $\rho = \rho_0$ (say), while as $x \to \infty$, far beyond the confining wall, $\rho = m_1 = m_2 = 0$. Restoring the Γ term we finally obtain Eq. (4) of the main text.

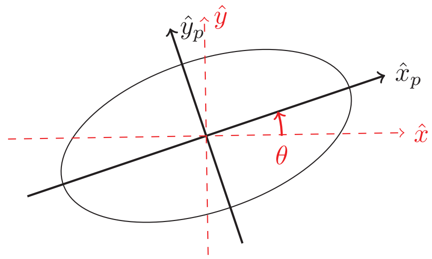

Figure 1. An illustration of the axes $(\hat{x}, \hat{x})$ and $(\hat{x}_p, \hat{x}_p)$, and the angle θ.

IV. PRESSURE FOR AN ELLIPSE IN A HARMONIC POTENTIAL

In what follows we first compute the torque applied on an ellipse in a harmonic potential. We then derive an approximate expression for the pressure, Eq. (5) of the main text, which is valid as long as the density distribution $P(r, \theta)$ equals its bulk value as soon as the wall potential vanishes (at $x = x_w$).

A. Torque on an ellipse

We consider an ellipse of uniform density and long and short axes of lengths a and b respectively. We define two sets of axes: 1) $(\hat{x}, \hat{y})$ are the real space coordinates with the wall parallel to the y axis, and 2) $(\hat{x}_p, \hat{y}_p)$ are the coordinates associated with the ellipse so that x_p is parallel to its long axis. The angle between the two sets of coordinates is θ, which is also the direction of motion of the particle (see Fig. 1). For simplicity, we assume that the particle is moving along its long principal axis.

Since the wall is perpendicular to the $\hat{x}$ axis, the force acting on an area element of the ellipse is given by $F_w(x_0 + x) = -\partial_x V(x_0 + x)$, where x_0 is the position of the center of mass of the ellipse and x the relative coordinate of the area element within the ellipse, both along the $\hat{x}$ direction.

The torque applied by the force at a point $\mathbf{r}$ is then given by

$$\gamma = \mathbf{r} \times F_w(x_0 + x)\hat{x} \ , \tag{9}$$

$$= \begin{pmatrix} x_p \\ y_p \end{pmatrix} \times F_w(x_0 + x_p \cos\theta - y_p \sin\theta) \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} \ . \tag{10}$$

Next, we integrate over the ellipse, taking its mass density to be uniform $\rho(x_p, y_p) = m/(\pi ab)$. Rescaling the axes as $x'_p = x_p/a$ and $y'_p = y_p/b$ to transform the ellipse into a unit circle, and switching from (x'_p, y'_p) to polar coordinates (r, φ), yields

$$\begin{aligned}\Gamma &= \frac{m}{\pi ab} \int dx_p dy_p \gamma \qquad (11)\\ &= \frac{m}{\pi} \int dx'_p \int dy'_p F_w(x_0 + ax'_p \cos\theta - by'_p \sin\theta) \begin{pmatrix} ax'_p \\ by'_p \end{pmatrix} \times \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix}\\ &= m \int_0^{2\pi} \frac{d\varphi}{\pi} \int_0^1 dr r F_w(x_0 + ar\cos\varphi\cos\theta - br\sin\varphi\sin\theta) \begin{pmatrix} ar\cos\varphi \\ br\sin\varphi \end{pmatrix} \times \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} \ .\end{aligned}$$

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For a harmonic wall potential $F_w(x) = -\lambda x$, the integral can be computed, and we get

$$\Gamma = \frac{m\lambda}{8}(a^2 - b^2)\sin(2\theta) \equiv \lambda\kappa\sin(2\theta) , \tag{12}$$

which has the expected symmetries: it vanishes for a sphere ($a = b$), and for particles moving along or perpendicular to the x-axis. Note that the torque is constant, independent of the position of the particle as long as the whole ellipse is within the range of the wall potential. In the main text we assume that this is always the case, which means that the ellipse is very small when compared to the typical decay length of $\rho(x)$ due to V. In the simulations, we thus simulated point-like ABPs with external torques $\Gamma = \pm\lambda\kappa\sin 2\theta$ for left and right walls. For real systems, the collision details would clearly be different, hence giving different quantitative predictions for the pressure P, but the qualitative results would be the same. We set $m = 1$ for ease of notation and define the asymetry coeficient $\kappa = (a^2 - b^2)/8$ as in the main text.

B. Approximate expression for the pressure

We now turn to the derivation of the approximate expression Eq. (5) in the main text for the pressure. In particular we focus on the case of ABP ($\alpha = 0$) ellipses confined by a harmonic wall potential and for simplicity neglect the translational diffusion $D_t = 0$. In that case the contribution of the torque to the pressure reads

$$C = \frac{\bar{\lambda}v}{\mu_t}\int_0^{+\infty} dx \int_0^{2\pi} d\theta \sin(\theta)\sin(2\theta)\mathcal{P}(x,\theta) , \tag{13}$$

where we have used expression (12) for Γ and defined $\bar{\lambda} = \mu_r\kappa\lambda/D_r$.

We will now expand the pressure P as a power series in $\bar{\lambda}$. If we make the approximation $P(x_w,\theta) = \rho_0/(2\pi)$, so that the steady-state distribution relaxes to its bulk value as soon as the system is outside the range of the wall potential, we can resum the series to obtain Eq. (5) of main text.

We first expand the probability distribution $\mathcal{P}(x,\theta)$ in powers of $\bar{\lambda}$

$$\mathcal{P}(x,\theta) = \sum_{k=0}^{\infty} \bar{\lambda}^k \mathcal{P}_k(x,\theta) , \tag{14}$$

so that the pressure is given by

$$P = \frac{v^2}{2\mu_t D_r}\rho_0 - C = \frac{v^2}{2\mu_t D_r}\rho_0 - \frac{v}{\mu_t}\sum_{k=0}^{\infty} C_k\bar{\lambda}^{k+1} , \tag{15}$$

where

$$C_k = \int_{x_w}^{\infty} dx \int_0^{2\pi} d\theta \sin\theta\sin(2\theta)\mathcal{P}_k(x,\theta) . \tag{16}$$

1. *Computation of the coefficients C_k*

C_0 is known since $\mathcal{P}_0 = \rho_0/2\pi$. Using the hypothesis $\mathcal{P}(x_w,\theta) = \rho_0/(2\pi)$, so that $\mathcal{P}_{k\geq 1}(x_w) = 0$, we can now relate $\mathcal{P}_k$ to $\mathcal{P}_{k-1}$ and then compute iteratively the C_k's.

In steady-state, the master equation gives for $x > x_w$, order by order in $\bar{\lambda}$:

$$0 = -\partial_x(v\cos\theta\mathcal{P}_k - \frac{\mu_t D_r}{\kappa\mu_r}(x - x_w)\mathcal{P}_{k-1}) + D_r\partial_\theta^2\mathcal{P}_k - D_r\partial_\theta(\sin(2\theta)\mathcal{P}_{k-1}), \quad k \geq 1 \tag{17}$$

$$0 = -\partial_x(v\cos\theta\mathcal{P}_0) + D_r\partial_\theta^2\mathcal{P}_0\ . \tag{18}$$

Multiplying Eq. (17) by an arbitrary function $f(\theta)$ and integrating over θ and x, one gets

$$\int_{x_w}^{\infty} dx \int_0^{2\pi} d\theta f''\mathcal{P}_k = -\int_{x_w}^{\infty} dx \int_0^{2\pi} d\theta f' \sin(2\theta)\mathcal{P}_{k-1}, \quad k \geq 1 \tag{19}$$

$$\int_{x_w}^{\infty} dx \int_0^{2\pi} d\theta f''\mathcal{P}_0 = -\frac{1}{D_r}\int_0^{2\pi} d\theta v\cos\theta f\mathcal{P}_0(x_w,\theta) = -\frac{v\rho_0}{2\pi D_r}\int d\theta\cos\theta f\ . \tag{20}$$

For conciseness, we define the operators T and T^*

$$T(f) = \sin(2\theta)\int d\theta f \quad , \qquad T^*(f) = \cos\theta\int d\theta\int d\theta f\ , \tag{21}$$

where the integral signs refer to indefinite integrals, to rewrite Eqs. (19-20) as

$$\int_{x_w}^{\infty} dx \int_0^{2\pi} d\theta g(\theta)\mathcal{P}_k = -\int_0^{\infty} dx \int_0^{2\pi} d\theta T(g(\theta))\mathcal{P}_{k-1}, \quad k \geq 1 \tag{22}$$

$$\int_{x_w}^{\infty} dx \int_0^{2\pi} d\theta g(\theta)\mathcal{P}_0 = -\frac{1}{D_r}\int_0^{2\pi} d\theta v T^*(g(\theta))\mathcal{P}_0(x_w,\theta) = -\frac{v\rho_0}{2\pi D_r}\int d\theta T^*(g(\theta))\ , \tag{23}$$

where $g = f''$. The C_k's then reduce to the explicit integrals

$$C_k = (-1)^{k+1}\frac{v\rho_0}{2\pi D_r}\int_0^{2\pi} d\theta T^* T^{k+1}(\cos\theta)\ , \tag{24}$$

where we use $\sin\theta\sin(2\theta) = T(\cos\theta)$ so that $T^k(\sin\theta\sin(2\theta)) = T^{k+1}(\cos\theta)$.

Let us now compute the C_k's. By inspection, one sees that $T^k(\cos\theta)$ is of the form

$$T^k(\cos\theta) = \sum_{i=0}^{k} \alpha_i^k \cos((2i+1)\theta)\ , \tag{25}$$

where the coefficients α_i^k obey the recursion

$$\alpha_0^0 = 1, \qquad \alpha_{j>0}^0 = 0\ , \tag{26}$$

$$\alpha_0^{k+1} = \frac{\alpha_0^k}{2} + \frac{\alpha_1^k}{6} \tag{27}$$

$$\alpha_i^{k+1} = \frac{1}{2}\left(\frac{\alpha_{i+1}^k}{2i+3} - \frac{\alpha_{i-1}^k}{2i-1}\right)\ , \tag{28}$$

$$\alpha_k^{k+1} = -\frac{1}{2}\frac{\alpha_{k-1}^k}{2k-1}\ , \tag{29}$$

$$\alpha_{k+1}^{k+1} = -\frac{1}{2}\frac{\alpha_k^k}{2k+1}\ , \tag{30}$$

which solution is

$$\alpha_j^k = \frac{(-1)^j}{k+1}\frac{(2j+1)}{(k+j+1)!}\prod_{i=0}^{j}(k+1-i)\ . \tag{31}$$

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After the application of T^* in Eq. (24), the only term that contributes to C_k in $T^k(\cos\theta)$ is $\alpha_0^k = \frac{1}{(k+1)!}$, because $\int d\theta \cos\theta \cos[(2i+1)\theta] = 0$ for $i > 0$. One thus finally gets

$$C_k = (-1)^k \frac{v\rho_0}{2\pi D_r} \int_0^{2\pi} d\theta \alpha_0^{k+1} \cos^2(\theta) = (-1)^k \frac{v\rho_0}{2D_r(k+2)!} . \tag{32}$$

2. *Approximate expression for the pressure*

The series (15) can now be resummed to yield

$$P = \frac{v^2}{2\mu_t D_r}\rho_0 \left(1 - \sum_{k=0}^{\infty}(-1)^k \frac{\bar{\lambda}^{k+1}}{(k+2)!}\right) = P_I \frac{1-e^{-\bar{\lambda}}}{\bar{\lambda}} , \tag{33}$$

where P_I is the ideal gas pressure. As expected, the pressure tends to P_I as $\bar{\lambda} \to 0$.

As can be seen in the right panel of Fig. 1 in the main text, the approximation that the wall does not affect the probability density for $x \leq x_w$ is not satisfied when $\bar{\lambda}$ is large. However, this happens only when $P(\bar{\lambda})$ is already very small, so that the analytic formula Eq. (33) compares very well with the $P(\bar{\lambda})$ curve obtained numerically, as shown in Figure 1 of main text.

V. NON–BOLTZMANN DISTRIBUTION

While the analytical computation of the full distribution for RTPs and ABPs in two dimensions is beyond the scope of this paper, here we show explicitly that the steady–state density is not a Boltzmann distribution for 1D RTPs. The master equation for the probability densities of right and left-movers ($\mathcal{P}_+(x,t)$ and $\mathcal{P}_-(x,t)$) is given by (see Ref. (26) of the main text)

$$\begin{aligned} \partial_t \mathcal{P}_+ &= -\partial_x \left(v - \mu_t \partial_x V\right) - \frac{\alpha}{2}\left(\mathcal{P}_+ - \mathcal{P}_-\right) , \\ \partial_t \mathcal{P}_- &= -\partial_x \left(-v - \mu_t \partial_x V\right) - \frac{\alpha}{2}\left(\mathcal{P}_- - \mathcal{P}_+\right) . \end{aligned} \tag{34}$$

Note that $D_t = 0$ for this system. The equation for the steady-state density then reads

$$\partial_x \left[\left(v^2 - \mu_t^2 (\partial_x V)^2\right)\rho\right] + \alpha\mu_t(\partial_x V)\rho = 0 . \tag{35}$$

First, rescale the potential so that the equation reduces to

$$\partial_x \left[\left(1 - (\partial_x \tilde{V})^2\right)\rho\right] + g(\partial_x \tilde{V})\rho = 0 , \tag{36}$$

with $g = \alpha/v$ and $\tilde{V} = V\mu_t/v$. The steady state distribution is then given by

$$\rho(x) = \rho_0 e^{-Q} , \tag{37}$$

and

$$Q = \ln[1 - (\partial_x \tilde{V}(x))^2] + \int_0^x dx' \frac{g\partial_{x'}\tilde{V}(x')}{1 - (\partial_{x'}\tilde{V}(x'))^2} . \tag{38}$$

The probability distribution is non-local inside the wall and not given by a Boltzmann distribution. (Note that particles are confined within the region $[0, x^*]$ where $(\partial_x \tilde{V})^2 < 1$ and $\rho(x) = 0$ outside.)

Despite the absence of a Boltzmann distribution, the pressure is well defined (as for the 2D case considered in the text). To see this explicitly in one dimension consider the expression for the pressure

$$P = \frac{v}{\mu_t} \int_0^{x^*} \partial_x V(x)\rho(x) \,, \tag{39}$$

with $\partial_x V(x^*) = 1$. Then using the explicit expression of the steady-state distribution, P can be written as

$$P = -\rho_0 \frac{v}{g\mu_t} \int_0^{x^*} dx \partial_x e^{-g\int_0^x dx' \frac{\partial_{x'} V(x')}{1-(\partial_{x'} V(x'))^2}} \,, \tag{40}$$

so that

$$P = -\rho_0 \frac{v}{g\mu_t} \left(e^{-g\int_0^{x^*} dx' \frac{\partial_{x'} V(x')}{1-(\partial_{x'} V(x'))^2}} - 1 \right) \,. \tag{41}$$

Now, since at the upper bound of the integral within the exponential the integrand diverges we have

$$P = \rho_0 \frac{v}{g\mu_t} = \rho_0 \frac{v^2}{\alpha\mu_t} \,. \tag{42}$$

VI. ANISOTROPIC PRESSURE

We consider spherical particles whose speeds depend on their direction of motion θ. As discussed in the main text, such situations could arise, for example, when the motion takes place on a corrugated surface. For simplicity, we consider only run–and–tumble particles ($D_r = 0$). The case of active Brownian particles can be treated following the same argument.

In steady–state, the master equation yields

$$0 = -\partial_x \left[\left(v(\theta)\cos\theta - \mu_t \partial_x V - D_t \partial_x \right) \mathcal{P}(\theta, \mathbf{x}) \right] - \alpha \mathcal{P} + \frac{\alpha}{2\pi} \int d\theta' \mathcal{P}(\theta', \mathbf{x}) \,. \tag{43}$$

We want to restrict ourselves to cases where the bulk currents along any direction vanish (the system is therefore uniform in the bulk), which we achieve by assuming that $v(\theta + \pi) = v(\theta)$. Following the same steps that lead to Eq. (4) in the main text, we get in steady state

$$0 = -\partial_x (\tilde{m}_1 - \mu_t \rho \partial_x V - D_t \partial_x \rho) \,, \tag{44}$$

$$0 = -\partial_x \left[\int_0^{2\pi} v(\theta)^2 \cos^2(\theta) \mathcal{P} d\theta - \mu_t \partial_x V \tilde{m}_1 - D_t \partial_x \tilde{m}_1 \right] - \alpha \tilde{m}_1 \,, \tag{45}$$

where we have defined $\tilde{m}_1 = \int_0^{2\pi} v(\theta)\cos(\theta)\mathcal{P} d\theta$ (which differs from m_1 in section III because it includes the speed).

From these two equations, we can express the mechanical pressure as a function of the bulk density and $v(\theta)$, as

$$P = \int_0^x \rho(x) \partial_x V dx = \frac{1}{\mu_t} \int_0^x (\tilde{m}_1 - D_t \partial_x \rho) = \left(\frac{D_t}{\mu_t} + \frac{\int_0^{2\pi} d\theta v^2(\theta)\cos^2(\theta)}{2\pi\alpha\mu_t} \right) \rho_0 \,. \tag{46}$$

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This holds for a wall perpendicular to the $\hat{x}$ axis. For a wall tilted by an angle ϕ, one obtains the anisotropic pressure

$$P(\phi) = \left(\frac{D_t}{\mu_t} + \frac{\int_0^{2\pi} d\theta v^2(\theta) \cos^2(\theta - \phi)}{2\pi\alpha\mu_t} \right) \rho_0 \ , \tag{47}$$

which is Eq. (9) of the main text.

VII. INTERACTING ACTIVE BROWNIAN PARTICLES

In the following we study ABPs with aligning interactions (Section VII A) and quorum-sensing interactions (Section VII B). In particular, we derive exact expressions for the pressure P in terms of microscopic correlators evaluated near the wall. These show P to depend explicitly on the details of the interaction with the wall, hence forbidding the existence of equations of state.

A. Aligning particles

We consider a system of N spherical ABPs which can exert torque on each other, for instance to promote the alignment of their directions of motion, but which do not feel any wall-torque. The positions and orientations of the particles evolve according to the Itō-Langevin equations

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v} - \mu_t \partial_x V + \sqrt{2D_t}\eta_i(t) \tag{48}$$

$$\frac{d\theta_i}{dt} = \mu_r \sum_j F(\theta_j - \theta_i, \mathbf{r}_i, \mathbf{r}_j) + \sqrt{2D_r}\xi_i(t) \tag{49}$$

where η_i and ξ_i are uncorrelated Gaussian white noises of unit variance and appropriate dimensionality. $F(\theta_j - \theta_i, \mathbf{r}_i, \mathbf{r}_j)$ is the torque exerted by particle j on particle i.

We now define a microscopic density field $\mathcal{P}(\mathbf{r}, \theta)$ as

$$\mathcal{P}(\mathbf{r}, \theta) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i)\delta(\theta - \theta_i) \tag{50}$$

Following [1], its evolution equation is given by

$$\partial_t \mathcal{P}(\mathbf{r}, \theta) = -\nabla \cdot [(\mathbf{v} - \mu_t \nabla V(x))\mathcal{P}(\mathbf{r}, \theta) - D_t \nabla \mathcal{P}(\mathbf{r}, \theta)] + \nabla \cdot \left(\sqrt{2D_t \mathcal{P}}\eta \right) + \partial_\theta \left(\sqrt{2D_r \mathcal{P}}\xi \right)$$
$$- \partial_\theta \left[\mu_r \int dr' \int_0^{2\pi} d\theta' F(\theta' - \theta, \mathbf{r}, \mathbf{r}')\mathcal{P}(\mathbf{r}, \theta)\mathcal{P}(\mathbf{r}', \theta') \right] + D_r \partial_\theta^2 \mathcal{P}(\mathbf{r}, \theta) \tag{51}$$

where the integral $\int d\mathbf{r}'$ is performed over all space.

We then follow the same reasoning as for non-interacting particles to derive an expression for the pressure. We first average Eq. (51) in steady-state, assuming translational invariance along y, to get

$$0 = -\partial_x [(\mathbf{v} - \mu_t \partial_x V(x))\langle \mathcal{P} \rangle - D_t \partial_x \langle \mathcal{P} \rangle] - \partial_\theta \left[\mu_r \int dr' \int_0^{2\pi} d\theta' F(\theta' - \theta, \mathbf{r}, \mathbf{r}') \langle \mathcal{P}(\mathbf{r}, \theta)\mathcal{P}(\mathbf{r}', \theta') \rangle \right]$$
$$+ D_r \partial_\theta^2 \langle \mathcal{P} \rangle \tag{52}$$

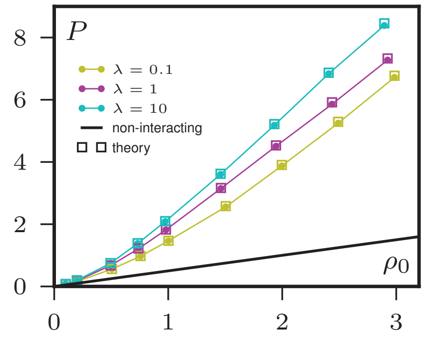

Figure 2. Lack of equation of state for ABPs with interparticle alignment interactions but no wall torques. The mechanical force per unit area P exerted on the wall is equal to its theoretical expression (56) and depends on the stiffness λ of the wall potential. The torque exerted by particle j on particle i is $F(\theta_j - \theta_i, \mathbf{r}_i, \mathbf{r}_j) = \frac{\gamma}{\mathcal{N}(\mathbf{r}_i)} \sin(\theta_j - \theta_i)$ if $|\mathbf{r}_j - \mathbf{r}_i| < R$ and 0 otherwise, where $\mathcal{N}(\mathbf{r}_i)$ is the number of particles interacting with particle i. ($v = 1$, $D_r = 1$, $D_t = 0$ and $\gamma = 2$.)

where the brackets $\langle \cdot \rangle$ denote averaging over noise realisations. Note that the noise terms average to zero due to our use of the Itō convention.

Multiplying Eq. (52) by 1 and $\cos\theta$ and then integrating over θ gives the analog of Eq. (6) and (7)

$$0 = -\partial_x[v m_1 - \mu_t \rho (\partial_x V) - D_t \partial_x \rho] \tag{53}$$

$$D_r m_1 = -\partial_x \left[v \frac{\rho + m_2}{2} - \mu_t m_1 (\partial_x V) - D_t \partial_x m_1 \right] - \mu_r \int_0^{2\pi} \sin\theta \int dr' \int_0^{2\pi} d\theta' F(\theta' - \theta, \mathbf{r}, \mathbf{r}') \langle \mathcal{P}(\mathbf{r}, \theta) \mathcal{P}(\mathbf{r}', \theta') \rangle \tag{54}$$

where $m_n(x) = \int_0^{2\pi} \cos(n\theta) \langle \mathcal{P}(x, \theta) \rangle d\theta$ and $\rho(x) = \int_0^{2\pi} \langle \mathcal{P}(x, \theta) \rangle d\theta$.

Inserting Eq. (54) in Eq. (53) allows us to rewrite the pressure $P = \int_0^\infty dx \rho \partial_x V$ exactly as

$$P = \left[\frac{v^2}{2\mu_t D_r} + \frac{D_t}{\mu_t} \right] \rho_0 - \frac{v \mu_r}{\mu_t D_r} \int_0^\infty dx \int_{-\infty}^\infty dy \int_0^{2\pi} d\theta \int d\mathbf{r}' \int_0^{2\pi} d\theta' F(\theta' - \theta, \mathbf{r}, \mathbf{r}') \sin\theta \langle \mathcal{P}(\mathbf{r}, \theta) \mathcal{P}(\mathbf{r}', \theta') \rangle \tag{55}$$

We see that, just as in Eq. (4) in main text, the mechanical pressure depends explicitly on the density $\mathcal{P}(\mathbf{r}, \theta)$ close to the wall, which in turn depends on the detail of the interaction $V(x)$ between the particles and the wall. There is thus no equation of state.

Using the microscopic definition of $\mathcal{P}$, Eq. (50), one can rewrite the integral in Eq. (55) as a sum over all particles, more suitable to numerical measurements:

$$P = \left[\frac{v^2}{2\mu_t D_r} + \frac{D_t}{\mu_t} \right] \rho_0 - \frac{v \mu_r}{\mu_t D_r} \langle \sum_{i,j=1}^N F(\theta_j - \theta_i, \mathbf{r}_i, \mathbf{r}_j) \sin\theta_i \Theta(x_i) \rangle \tag{56}$$

where $\Theta(x_i) = 1$ if $x_i > 0$ and zero otherwise. In Fig. 2, we compare measurements of P from the force applied on the confining wall and from Eq. (56), for a particular choice of F. They show perfect agreement, thus confirming Eq. (55).

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B. Quorum-sensing interactions

A similar path can be followed to compute the pressure exerted by ABPs that adapt their swim speed to the local density computed through a coarse-graining kernel $\bar{\rho}(\mathbf{r}) = \sum_i K(|\mathbf{r}-\mathbf{r}_i|)$, where the sum runs over all particles. The dynamics of the system is now given by the Itō-Langevin equations

$$\frac{d\mathbf{r}_i}{dt} = v(\bar{\rho})\mathbf{e}_i - \mu_t \partial_x V + \sqrt{2D_t}\eta_i(t) \tag{57}$$
$$\frac{d\theta_i}{dt} = \sqrt{2D_r}\xi_i(t) \tag{58}$$

As before, the dynamics of the density field can be obtained using Itō calculus [1]

$$\begin{aligned}\partial_t \mathcal{P}(\mathbf{r},\theta) = -\nabla\cdot[(v(\bar{\rho})\mathbf{e}_\theta - \mu_t\nabla V(x))\mathcal{P}(\mathbf{r},\theta) - D_t\nabla\mathcal{P}(\mathbf{r},\theta)] + D_r\partial_\theta^2\mathcal{P}(\mathbf{r},\theta)\\ + \nabla\cdot\left(\sqrt{2D_t\mathcal{P}}\eta\right) + \partial_\theta\left(\sqrt{2D_r\mathcal{P}}\xi\right)\end{aligned} \tag{59}$$

By the same procedure as for aligning particles (except that we first multiply Eq. (59) by $v(\bar{\rho})$ for the second equation) we get the two relations

$$0 = -\partial_x[\langle v(\bar{\rho})\hat{m}_1\rangle - \mu_t\rho(\partial_x V) - D_t\partial_x\rho] \tag{60}$$
$$D_r\langle v(\bar{\rho})\hat{m}_1\rangle = -\left\langle v(\bar{\rho})\partial_x\left[v(\bar{\rho})\frac{\hat{\rho}+\hat{m}_2}{2} - \mu_t\hat{m}_1(\partial_x V) - D_t\partial_x\hat{m}_1\right]\right\rangle \tag{61}$$

where $\hat{m}_n(x) = \int_0^{2\pi}\cos(n\theta)\mathcal{P}(x,\theta)d\theta$ and $\hat{\rho}(x) = \int_0^{2\pi}\mathcal{P}(x,\theta)d\theta$ are fluctuating quantities whose averages are m_n and ρ.

We can now rewrite the pressure using these two equalities:

$$P = \int_0^\infty dx\rho\partial_x V = \frac{1}{\mu_t}\int_0^\infty dx\left[\langle v(\bar{\rho})\hat{m}_1\rangle - D_t\partial_x\rho\right] \tag{62}$$
$$= \frac{D_t}{\mu_t}\rho_0 - \frac{1}{D_r\mu_t}\int_0^\infty dx\left\langle v(\bar{\rho})\partial_x\left[v(\bar{\rho})\frac{\hat{\rho}+\hat{m}_2}{2} - \mu_t\hat{m}_1(\partial_x V) - D_t\partial_x\hat{m}_1\right]\right\rangle \tag{63}$$

Integrating by part the last integral, we obtain

$$\begin{aligned}P = &\frac{\langle v(\bar{\rho})^2(\hat{\rho}+\hat{m}_2)\rangle_0}{2\mu_t D_r} - \frac{D_t\langle v(\bar{\rho})\partial_x\hat{m}_1\rangle\rangle_0}{\mu_t D_r} + \frac{D_t}{\mu_t}\rho_0\\ &+ \frac{1}{D_r\mu_t}\int_0^\infty dx\left\langle \partial_x v(\bar{\rho})\left[v(\bar{\rho})\frac{\hat{\rho}+\hat{m}_2}{2} - \mu_t\hat{m}_1(\partial_x V) - D_t\partial_x\hat{m}_1\right]\right\rangle\end{aligned} \tag{64}$$

where the brackets $\langle\cdot\rangle_0$ denote an average done in the bulk of the system.

As for aligning particles, one can use Eq. (50) to obtain a "microscopic expression" for P which is more suitable for numerical evaluation:

$$\begin{aligned}P = &\frac{D_t}{\mu_t}\rho_0 + \sum_{i=1}^N\left(\frac{\langle v(\bar{\rho}_i)^2(1+\cos(2\theta_i))\rangle_0}{2\mu_t D_r} + \frac{2D_t\langle\partial_{x_i}v(\bar{\rho}_i)\cos\theta_i\rangle_0}{\mu_t D_r}\right)\\ &+ \sum_{i=1}^N\Theta(x_i)\frac{1}{D_r\mu_t}\left\langle\partial_{x_i}v(\bar{\rho}_i)\left[v(\bar{\rho}_i)\frac{1+\cos(2\theta_i)}{2} - \mu_t\cos\theta_i(\partial_x V)\right] + D_t(\partial_{x_i}^2 v(\bar{\rho}_i))\cos\theta_i\right\rangle\end{aligned} \tag{65}$$

Here, for ease of notation, we have written $\bar{\rho}_i = \bar{\rho}(\mathbf{r}_i)$. Again this exact formula shows that no equation of state relates the mechanical pressure to bulk properties of the system.

[1] Farrell, F. D. C., Tailleur, J., Marenduzzo D. and Marchetti M. C. , Pattern formation in self-propelled particles with density-dependent motility, Phys. Rev. Lett. **108**, 248101 (2012)