Supplemental Material: Rectification of Confined Soft Vesicles Containing Active Particles

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I. MEAN SQUARED DISPLACEMENT OF SOFT VESICLE CONTAINING ACTIVE PARTICLES

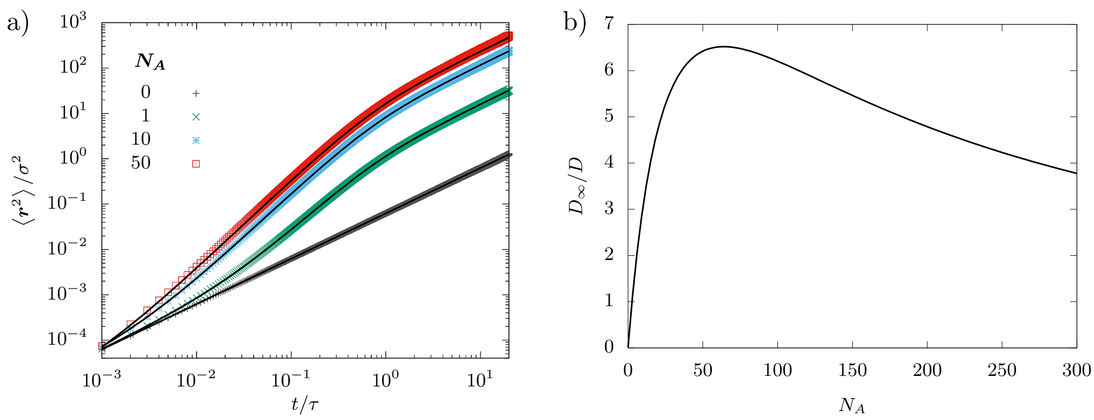

FIG. 1: a) Mean squared displacement of center of mass of a vesicle containing active particles. With no active particles, the motion remains diffusive at all times. With a finite number of active particles enclosed, the vesicle has a ballistic regime at $t \approx \tau$ and is diffusive for $t \gg \tau$. The solid black lines are the closed form expression from Eq. 4. b) The long time diffusion constant (Eq. 6) is non-monotonic and attains maximal value when the number of active particles N_A in the vesicle equals the number of colloids forming the flexible boundary of the vesicle N. Here, $N = 64$.

In this section, we evaluate the closed form expression for the mean squared displacement of the center of mass of the soft vesicle. This calculation follows the procedure adopted for run-and-tumble active particles within a vesicle [1]. The center of mass of the vesicle is defined as,

$$\boldsymbol{r}_{\rm cm} = \frac{1}{N+N_A}\left(\sum_{i=1}^{N}\boldsymbol{r}_i + \sum_{j=1}^{N_A}\boldsymbol{r}_j\right), \tag{1}$$

where $\boldsymbol{r}_i, \boldsymbol{r}_j$ denote the positions of the particles in the flexible boundary and the enclosed active colloids respectively. The velocity of the center of mass $\boldsymbol{v} = d\boldsymbol{r}/dt$ can be written explicitly in terms of the constituent particle velocities as,

$$\boldsymbol{v}_{\rm cm} = \frac{1}{N+N_A}\left(\sum_{i=1}^{N}\boldsymbol{v}_i + \sum_{j=1}^{N_A}\boldsymbol{v}_j\right). \tag{2}$$

The dynamics of the particle velocities is encoded in the Brownian equations of motion in Eq. 1 in the main text. The total force on the center of mass is the sum of all forces on all particles and given the symmetry of the problem the interaction forces between colloids add to zero [1]. We integrate the equations of motion of the colloidal particles to find the position of the center of mass,

$$\boldsymbol{r}_{\rm cm}(t) = \frac{1}{N+N_A}\left(\sqrt{2D}\sum_{i=1}^{N}\int_0^t \boldsymbol{\xi}_i(t')\,dt' + \sqrt{2D}\sum_{j=1}^{N_A}\int_0^t \boldsymbol{\xi}_j(t')\,dt' + v_p\sum_{j=1}^{N_A}\int_0^t \boldsymbol{n}_j(t')\,dt'\right). \tag{3}$$

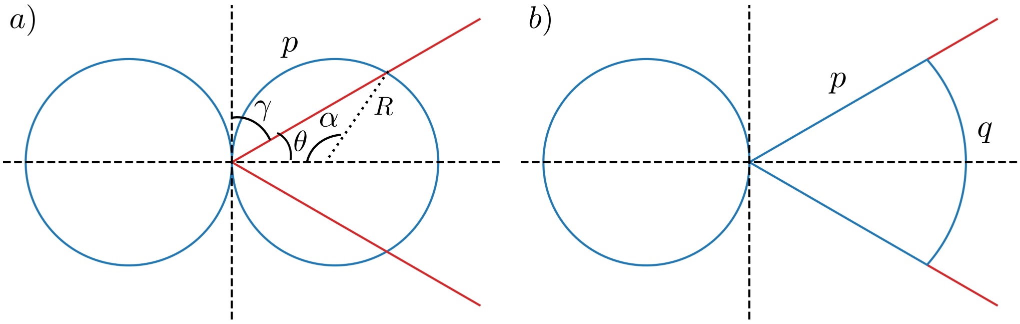

FIG. 2: Geometries used to calculate $P^L(\gamma)$. We ignore the finite pore width. In (b), we assume the length of the ring in contact with the wall p to be the same as the arc length in (a).

The mean squared displacement of the vesicle is,

$$\langle \boldsymbol{r}_{\rm cm}^2(t) \rangle = \frac{1}{(N+N_A)^2} \left(2D \sum_{i=1}^{N} \int_0^t \int_0^t \langle \boldsymbol{\xi}_i(t') \cdot \boldsymbol{\xi}_i(t'') \rangle \, dt' dt'' + 2D \sum_{i=j}^{N_A} \int_0^t \int_0^t \langle \boldsymbol{\xi}_j(t') \cdot \boldsymbol{\xi}_j(t'') \rangle \, dt' dt'' \right.$$
$$\left. + v_p^2 \sum_{j=1}^{N_A} \int_0^t \int_0^t \langle \boldsymbol{n}_j(t') \cdot \boldsymbol{n}_j(t') \rangle \; dt' dt'' \right) . \tag{4}$$

Given that noise on the colloidal particles is not correlated with each other and that the system is confined to two dimensions, we have $\langle \boldsymbol{\xi}_i(t') \cdot \boldsymbol{\xi}_i(t'') \rangle = 2\,\delta(t' - t'')$. The first two sets of integrals in Eq. 4 can be done employing the Dirac delta function. The third set of integrals involving the time-correlation of the orientation unit vector is evaluated following Hagen et al. [2]. The ensemble of active particles considered in [2] has a fixed initial direction of self-propulsion, which contributes direction specific terms to the mean squared displacement. However, since we numerically calculate the mean squared displacement of the vesicle along a trajectory, these terms average out to zero. Following the evaluation of the integrals in Eq. 4, we are able to write the mean squared displacement of the center of mass of the vesicle confined to two dimensions as,

$$\langle \boldsymbol{r}_{\rm cm}^2(t) \rangle = \frac{4D\,t}{N+N_A} + \frac{2\,Pe^2\sigma^2 N_A}{9\,(N+N_A)^2} \left(e^{-D_r\,t} + D_r\,t - 1 \right) . \tag{5}$$

The numerical results are tested against this expression in Fig. 1(a). The long time diffusion constant D_∞ defined as,

$$D_\infty = \lim_{t\to\infty} \frac{1}{4t} \langle \boldsymbol{r}_{\rm cm}^2(t) \rangle = \frac{D}{N+N_A} + \frac{Pe^2\sigma^2 N_A D_r}{18(N+N_A)^2}, \tag{6}$$

is non-monotonic as a function of N_A (See Fig. 1b). The number of active particles N_A^0 needed to attain the maximal D_∞ is calculated by setting the derivative of D_∞ with respect to N_A to be zero. This condition can be simplified to,

$$\frac{N_A^0}{N+N_A^0} = \frac{1}{2} - \frac{3}{Pe^2}. \tag{7}$$

For $Pe \to \infty$, $N_A^0 = N$.

II. PREFERENTIAL MOTILITY OF A VESICLE STUCK BETWEEN SLOPED WALLS

In this section, we estimate the probability of leftward transitions $P^L(\gamma)$ (Eq. 3 of main text) for the system in the inset of Fig. 3 of main text. We approximate the soft vesicle as two rings of equal radius R whose perimeters are $2\pi R$ each. We also ignore the finite pore width and set it to zero to allow for a simple calculation. See Fig. 2(a). The angle γ quantifies the slope of the slanted wall with respect to the $y-$ axis. The wall bisects the right side ring at two points. The angle bisected by the arc between these two points is α, and the arc length is $p = R\alpha$. We assume that for $N_A \gg 1$, the ring conforms to the wall as in Fig. 2(b), where the portion of the ring in contact with the wall is taken to be p. The length of curved portion of the right ring is $q = 2\pi R - 2p = 2R(\pi - \alpha)$. From the geometry of the system, we have $\alpha = \pi - 2\theta$ and $\theta = \pi/2 - \gamma$. In the high Pe limit, all particles are expected to be at the vesicle boundary. The number of active particles at the vesicle boundary is proportional to the length of the vesicle, and the force on the ring scales with the number of active particles. The probability of leftward transition is then,

$$P^L = \frac{2\pi R}{2\pi R + q}.$$

While all the active particles on the left ring push the vesicle leftwards, only the active particles on the free curved portion of the right ring push the vesicle rightwards. Using the geometric relations discussed above, P^L as a function of the angle γ can be found to be,

$$P^L(\gamma) = \frac{1}{2(1 - \gamma/\pi)}, \tag{8}$$

which is Eq. 3 of the main text.

[1] M. Paoluzzi, R. Di Leonardo, M. C. Marchetti and L. Angelani, *Scientific reports*, 2016, **6**, 1–10.
[2] B. ten Hagen, S. van Teeffelen and H. Löwen, *Condensed Matter Physics*, 2009, **12**, 725–738.