Entropy production of an active particle in a box
Supplemental Material

Nitzan Razin[1]

[1] *Division of Biology and Bioengineering, California Institute of Technology, Pasadena, California 91125, USA*

(Dated: September 19, 2020)

1. NO DIFFUSION ($D \to 0$) LIMIT OF THE STEADY STATE DISTRIBUTION

A. Taking the $D \to 0$ limit of the steady state density Eq. 3

As $D \to 0$, the length scale of wall accumulation $\xi \to 0$, yet the number of particles accumulated near the wall remains finite - resulting in a diverging particle density. We first derive an expression for the asymptotic behavior of $\rho(x)$ for small D. Since $\mathrm{Pe} \gg 1$, $\xi = \frac{\ell_p}{\mathrm{Pe}} + O(\mathrm{Pe}^{-2})$. Using this and $\xi \ll d$, we get:

$$\rho(x) \simeq \frac{1}{2(d+\ell_p)}\left(1 + \mathrm{Pe}\exp\left(\frac{|x|-d}{\xi}\right)\right) \tag{S1}$$

Taking the limit $\xi \to 0$, and using the identity $\lim_{\epsilon\to 0}\frac{1}{2\epsilon}e^{|x|/\epsilon} = \delta(x)$, we obtain:

$$\lim_{D\to 0}\rho(x) = \frac{1}{2(d+\ell_p)}\left(1 + 2\ell_p\delta(|x|-d)\right) \tag{S2}$$

where in order to maintain the particle number conservation normalization condition $\int_{-d}^{d}\rho(x)\mathrm{d}x = 1$, we define an integral over a delta function with the integration boundary at the point of the delta divergence to be equal to 1/2: $\int_0^a \delta(x) = \frac{1}{2}$ for $a > 0$ (consistent with the contribution of the asymptotic expression for small ξ to the integral).

Thus Eq. S2 describes a constant bulk density $\rho(x) = \frac{1}{2(d+\ell_p)}$ for $-d < x < d$, and a macroscopic particle number accumulated on each of the walls:

$$N^{-d} = \frac{\ell_p}{d+\ell_p}\lim_{\epsilon\to 0}\int_{-d}^{-d+\epsilon}\mathrm{d}x\,\delta(|x|-d) = \frac{\ell_p}{2(d+\ell_p)} \tag{S3}$$

and similarly the number of particles at $x = d$ is $N^d = N^{-d}$, where we denote the number of particles at $x = \pm d$ by N^x.

B. Solving coupled equations directly for $D = 0$

The coupled rate equations for the bulk density of left and right moving particles, and for the numbers of particles accumulated on the walls:

$$\begin{aligned}
\partial_t R &= -\partial_x J_R + \tfrac{\alpha}{2}(L-R)\\
\partial_t L &= -\partial_x J_L + \tfrac{\alpha}{2}(R-L)\\
\partial_t N_L^{-d} &= -J_L(-d) - \tfrac{\alpha}{2}N_L^{-d}\\
\partial_t N_R^{-d} &= -J_R(-d) + \tfrac{\alpha}{2}N_L^{-d}\\
\partial_t N_L^{d} &= J_L(d) + \tfrac{\alpha}{2}N_R^{d}\\
\partial_t N_R^{d} &= J_R(d) - \tfrac{\alpha}{2}N_R^{d},
\end{aligned} \tag{S4}$$

where $J_R(x,t) = vR(x,t)$ and $J_L = -vL(x,t)$ are the currents of right and left moving particles, and $N_{L/R}^x$ is the number of left/right-moving particles at the boundary position $x = \pm d$. The number of particles accumulated on a wall that are moving away from it is zero (i.e. $N_R^{-d} = N_L^d = 0$). We set the total particle number to 1: $\int_{-d}^{d}\rho(x)\mathrm{d}x + N_L^{-d} + N_R^d = 1$, where $\rho(x) = R(x) + L(x)$ is the total particle density. The steady state solution of Eq. S4 is then

$$\begin{aligned}
&\rho(x) \equiv \rho_0 = \tfrac{1}{2(d+\ell_p)}\\
&R(x) = L(x) = \tfrac{1}{2}\rho_0\\
&N_L^{-d} = N_R^d = \tfrac{\ell_p}{2(d+\ell_p)},\ N_R^{-d} = N_L^d = 0
\end{aligned} \tag{S5}$$

This is the same as the solution derived in the previous subsection by taking the $D \to 0$ limit of the steady state density. More general versions of these equations allowing position dependent v and α, and including sink and source terms, have analytic steady state solutions that were studied in [1, 2].

2. MAXIMUM OF THE ENTROPY PRODUCTION RATE DERIVATIVE $\partial_d\Pi$

We show below that the entropy production rate derivative as a function of the system size, $\partial_d\Pi(d;\alpha,\xi,\mathrm{Pe})$, is maximal at $d_{\max} = \xi f(\mathrm{Pe})$ where

$$f(\mathrm{Pe}) \simeq \begin{cases}\text{constant} \approx 0.91, & \text{if } \mathrm{Pe} \ll 1\\ -\frac{1}{2}W_{-1}(\frac{1}{2\mathrm{Pe}}), & \text{if } \mathrm{Pe} \gg 1\end{cases} \tag{S6}$$

with $W_{-1}(x)$ being the -1 branch of the Lambert W function.

We defined the model by the FP equations Eq. 1 in terms of 4 independent parameters: the speed v, the tumble rate α, the diffusion coefficient D and the system half size d. We now study the change in entropy production

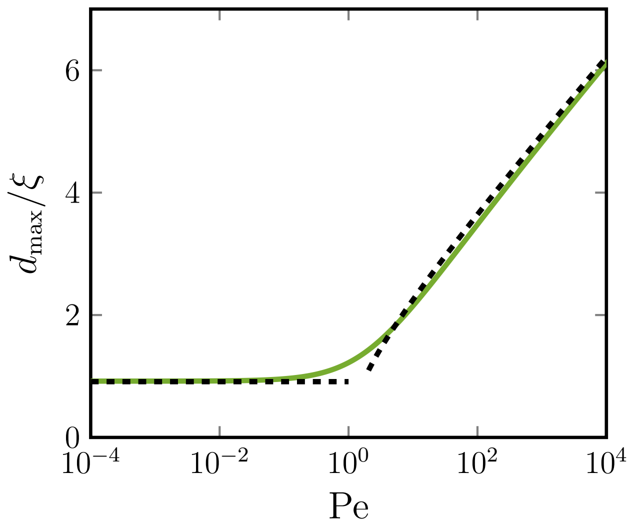

FIG. S1. The maximum point $d_{\max}$ of the entropy production rate derivative $\partial_d \Pi(d;\alpha,\xi,\mathrm{Pe})$ (Eq. S7). The ξ normalized maximum point $d_{\max}/\xi = f(\mathrm{Pe})$ is independent of α and ξ, and its dependence on Pe is plotted from numerical calculation (green line). The dashed black lines are analytic results for the asymptotic behavior of $f(\mathrm{Pe})$ in the $\mathrm{Pe} \ll 1$ and $\mathrm{Pe} \gg 1$ limits (Eq. S6).

rate Π as d is varied, as a function of an alternative set of 4 independent parameters, which instead of D and v includes the dimensionless Peclet number Pe, and the accumulation length scale ξ arising from the steady state density (Eq. 3).

The derivative of the EPR Π with respect to the system half length d:

$$\begin{aligned}\partial_d \Pi &= \frac{\alpha \mathrm{Pe}(1+\mathrm{Pe})\left(\sinh(\frac{2d}{\xi}) - 2\frac{d}{\xi}\right)}{2\xi\left(\frac{d}{\xi}\cosh(\frac{d}{\xi}) + \mathrm{Pe}\sinh(\frac{d}{\xi})\right)^2} \\ &= \frac{\alpha \mathrm{Pe}(1+\mathrm{Pe})}{2\xi} g(\tilde{d}, \mathrm{Pe}) \end{aligned} \tag{S7}$$

where we denote $\tilde{d} \equiv \frac{d}{\xi}$. $\partial_d \Pi$ has a single maximum as a function of d (Fig. 4b). From the form of Eq. S7, the maximum point $d_{\max} = \underset{d}{\mathrm{argmax}} \partial_d \Pi = \xi \tilde{d}_{\max}$ for $\tilde{d}_{\max} = \underset{\tilde{d}}{\mathrm{argmax}} g(\tilde{d}, \mathrm{Pe}) \equiv f(\mathrm{Pe})$ independent of α and ξ.

A numerical evaluation of $\tilde{d}_{\max}$ is plotted in Fig. S1. It appears that $f(\mathrm{Pe})$ has distinct behaviours in the two regimes $\mathrm{Pe} \ll 1$ and $\mathrm{Pe} \gg 1$. We shall perform a self-consistent analytic approximation of $\tilde{d}_{\max} = f(\mathrm{Pe})$ in each of these regimes.

First, in the $\mathrm{Pe} \ll 1$ limit, it seems that $\tilde{d}_{\max}$ converges to a constant which is slightly smaller than 1. In this limit,

$$g(\tilde{d}, \mathrm{Pe}) \simeq \frac{\left(\sinh(2\tilde{d}) - 2\tilde{d}\right)}{\tilde{d}^2 \cosh^2(\tilde{d})} \tag{S8}$$

Taking a 2nd order Taylor expansion around $\tilde{d} = 1$ and calculating the maximum of the resulting parabola gives $\tilde{d}_{\max} \approx 0.91$, consistent with the Taylor approximation assumption.

Next, consider the $\mathrm{Pe} \gg 1$ limit. From Fig. S1, in this limit $\tilde{d}_{\max}$ grows logarithmically with Pe. Thus we will look for an approximate solution for $\tilde{d}_{\max}$ when $\mathrm{Pe} \gg \tilde{d} \gg 1$. Using the approximation $\sinh(x) \approx \cosh(x) \approx \frac{1}{2}e^x$ for $x \gg 1$, we obtain:

$$g(\tilde{d}, \mathrm{Pe}) \simeq \frac{2\left(1 - 4\tilde{d}e^{-2\tilde{d}}\right)}{\left(\tilde{d} + \mathrm{Pe}\right)^2} \tag{S9}$$

Looking for a maximum by demanding that $\partial_{\tilde{d}} g(\tilde{d}) = 0$, and keeping only leading order terms for $\mathrm{Pe} \gg x \gg 1$, gives the demand $e^{2\tilde{d}} = 4\tilde{d}\mathrm{Pe}$. The solution of this equation is

$$\tilde{d}_{\max} = -\frac{1}{2} W_{-1}\left(\frac{1}{2\mathrm{Pe}}\right) \tag{S10}$$

where $W_{-1}(x)$ is the -1 branch of the Lambert W function. The results of the two approximations of the asymptotic behavior of $\tilde{d}_{\max}$ are plotted in Fig. S1, showing that the numerical evaluation of the maximum converges to the approximate results in the respective limits.

[1] N. Razin, R. Voituriez, J. Elgeti, and N. S. Gov, Phys. Rev. E **96**, 032606 (2017).

[2] N. Razin, R. Voituriez, J. Elgeti, and N. S. Gov, Phys. Rev. E **96**, 052409 (2017).