

Entropy Production in a Current-Free System

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We derive the leading-order contribution to the entropy production of two current-free systems in closed form. Both systems are derived from a one-dimensional Run-and-Tumble (RnT) particle with a hidden degree of freedom. These are the first examples of a closed-form expression for the entropy production rate of non-Markov systems. We furthermore develop a perturbation theory to systematically calculate the entropy production rates of processes operating in continuous space and time with hidden degrees of freedom. In particular, our method enables the calculation of the entropy production rate of irreversible processes with no net current.

I. INTRODUCTION

A pressing open question in the field of active matter concerns the possibility of extracting useful work from self-propelled particles, which include bacteria such as *E. Coli* or synthetic colloids. The key quantity of relevance in determining the maximum possible power which can be extracted from a system is the entropy production rate (*Good reference for this??*). Significant efforts have already been made to calculate the entropy production rates of a wide range of models of physical systems *Bunch of references here*. In all works referenced here, it is assumed that observers have complete access to all dynamical degrees of freedom in their models, which renders the systems Markovian.

Real systems are more complicated. Observers usually lack information about some hidden set of degrees of freedom, which may vary stochastically at inaccessibly short time and length scales. Upon removal of an observer's access to a subset of the total degrees of freedom, the behaviour of the remaining degrees of freedom becomes non-Markov, despite the fact that the underlying dynamics remain unchanged. Previous formulations of the entropy production rate have been unable to deal with

Stochastic thermodynamics provides a framework for extending extensive thermodynamic quantities such as work, heat, and energy to microscopic and mesoscopic systems. Such systems are commonly found in the context of active matter, as well as in biological tissue modelling and quantum mechanics. The entropy production of such systems has been the subject of particular interest. The entropy production distinguishes systems on their path to equilibrium, and those with fluctuations around the equilibrium state, from ensembles that exhibit true Non-Equilibrium Steady States (NESS). This characterisation is crucial to understanding the nature of energy dissipation in any system. For systems far-from-equilibrium, the entropy production governs the rate of approach to equilibrium through the relevant fluctuation theorem. Moreover, the entropy production bounds the free energy cost of maintaining a process, see for example [1, 2] for discussions on the relationship between heat flow and the energy cost of embryonic processes.

For systems driven by Markovian dynamics the rate of entropy production can be deduced from the master equation (discrete state-space) or the Langevin equation (continuous state-space). Examples of Markovian systems whose entropy productions can be exactly solved can be found in the context of molecular engines, chemical reactions, and quantum systems [3]. While many different schemes for the entropy production of non-Markovian systems have been studied, a survey of the literature reveals no reference models.

Here we derive a perturbative expression for the entropy production of a diffusion process whose self-propulsion rate is governed by a hidden stochastic process independent of the noise. This hidden degree of freedom renders the process non-Markov. We apply this result to obtain the first-order contribution to the entropy production when the hidden process is an asymmetric telegraph process. We also extend to the case where the diffusion process is confined in a harmonic potential. To the authors' knowledge, this is the first example of a closed form expression for the entropy production of a non-Markovian process.

...end intro ...

A case of particular interest is when $w(t)$ follows a telegraph process (FIND CITATION), switching between two values w_1 and w_2 with Poissonian rates α_1 and α_2 respectively (INSERT FIGURES HERE - two state process with arrows and rates, and typical w trajectory).

We consider the situation where an observer of this process only has knowledge of the trajectory of the particle in position space, denoted $\{\dot{x}(t)\}$, and not of the telegraph process $w(t)$. Given this incomplete description the process is no longer Markov. This is because, letting τ be a time increment such that $\alpha_1\tau, \alpha_2\tau \ll 1$, the net movement of the particle in time τ is strongly correlated with the instantaneous state of the hidden variable $w(t)$. The probability of the path $\{\dot{x}(t)\}$ having occurred is denoted by $\mathcal{P}[\{\dot{x}(t)\}]$. When the trajectory of the self propulsion velocity $\{w(t)\}$ is also known to the observer, the subsequent evolution of ...

The observable of interest is the entropy production rate, which measures the distance of a process from equilibrium. It is given by (REFERENCE GASPARD)

$$\dot{S} = \lim_{T \rightarrow \infty} \frac{1}{T} \left\langle \ln \left(\frac{\mathcal{P}[\{\dot{x}\}]}{\mathcal{P}[\{\dot{x}\}^R]} \right) \right\rangle \quad (1)$$

II. DERIVATION OF ENTROPY PRODUCTION RATE

Consider a self-propelling particle whose motion is described by the Langevin equation

$$\begin{aligned} \dot{x}(t) &= \nu w(t) - \frac{\partial V}{\partial x} + \xi(t) \\ \langle \xi(t)\xi(t') \rangle &= 2D\delta(t-t') \end{aligned} \quad (2)$$

where $x(t)$ and $w(t)$ are the position and self-propulsion velocity of the particle respectively, ν is a dimensionless bookkeeping parameter, $V = V(x)$ is a potential expressed in units of velocity, and $\xi(t)$ represents white noise with diffusion constant D .

We seek to express the probability of a specific realisation of a velocity trajectory $\{\dot{x}(t)\}$ occurring as a result of the dynamics (2). It is first assumed that the trajectory of the self-propulsion $\{w(t)\}$ is known. Using the fact that the noise $\xi(t)$ follows a Gaussian distribution (Onsager-Machslup(ref?))

$$\mathcal{P}[\{\dot{x}(t)\}|\{w(t)\}] \propto \exp \left\{ -\frac{1}{4D} \int dt \left(\dot{x} + \frac{\partial V}{\partial x} - \nu w \right)^2 \right\} \quad (3)$$

By marginalising over all possible trajectories $\{w(t)\}$, we arrive at the probability of the realisation of a spatial path $\{\dot{x}(t)\}$, $\mathcal{P}[\{\dot{x}(t)\}]$ ~~which makes no reference to a trajectory of the self-propulsion velocity $w(t)$~~ . Introducing the following notation for clarity:

$$\bar{\bullet} = \int \mathcal{D}w(t) \mathcal{P}[\{w(t)\}] \bullet \quad (4)$$

the spatial path probability may be expressed from equation (3) as

$$\begin{aligned} \mathcal{P}[\{\dot{x}(t)\}] &= \overline{\overline{\mathcal{P}[\{\dot{x}(t)\}|\{w(t)\}]}} \\ &= \exp \left(-\frac{1}{4D} \int dt (\dot{x} + V')^2 \right) \overline{\overline{\exp \left(-\frac{1}{4D} \int dt (-2\dot{x}\nu w - 2\nu w V' + (\nu w)^2) \right)}} \end{aligned} \quad (5)$$

A. Perturbation Theory

We proceed by expanding perturbatively in the dimensionless velocity coefficient ν :

$$\begin{aligned} \mathcal{P}[\{\dot{x}(t)\}] = & \exp\left(-\frac{1}{4D} \int dt (\dot{x} + V')^2\right) \left[1 + \frac{\nu}{2D} \int dt \overline{w(t)} (\dot{x}(t) + V')\right. \\ & + \nu^2 \left(-\frac{1}{4D} \int dt \overline{w^2(t)} + \frac{1}{8D^2} \int dt_1 dt_2 \overline{w(t_1)w(t_2)} (\dot{x}(t_1)\dot{x}(t_2) + 2\dot{x}(t_1)V' + (V')^2)\right) \\ & \left. + \nu^3 \left(-\frac{1}{8D^2} \int dt_1 dt_2 \overline{w^2(t_1)w(t_2)} (\dot{x}(t_1) + V') + \frac{1}{48D^3} \int dt_1 dt_2 dt_3 \overline{w(t_1)w(t_2)w(t_3)} \prod_{i=1}^3 (\dot{x}(t_i) + V')\right) + \mathcal{O}(\nu^4)\right] \end{aligned} \quad (6)$$

This allows us to express the average entropy production rate of a *specific trajectory* $\{\dot{x}(t)\}$ of duration T (REFERENCE):

$$\begin{aligned} \dot{\mathcal{S}}(\{\dot{x}(t)\}) = & \frac{1}{T} \ln\left(\frac{\mathcal{P}[\{\dot{x}(t)\}]}{\mathcal{P}[\{\dot{x}(t)\}^R]}\right) \\ = & -\frac{1}{TD} \int_0^T \dot{x}(t)V' dt + \frac{\nu}{TD} \int_0^T dt \dot{x}(t) \overline{w(t)} \\ & - \frac{\nu^2}{T} \frac{1}{2D^2} \int_0^T dt_1 dt_2 \overline{w(t_1)w(t_2)} \dot{x}(t_1)V' \\ & + \frac{\nu^3}{T} \left[\frac{1}{4D^2} \int_0^T dt_1 dt_2 \overline{w(t_1)} \cdot \overline{w(t_2)^2} \dot{x}(t_1) + \frac{1}{24D^3} \int_0^T dt_1 dt_2 dt_3 \overline{w(t_1)w(t_2)w(t_3)} (\dot{x}(t_1)\dot{x}(t_2)\dot{x}(t_3) + 3\dot{x}(t_1)(V')^2) \right. \\ & \left. - \frac{1}{8D^3} \int_0^T \overline{w(t_1)} \cdot \overline{w(t_2)w(t_3)} (\dot{x}(t_1)\dot{x}(t_2)\dot{x}(t_3) + 3\dot{x}(t_1)(V')^2) \right] + \mathcal{O}(\nu^4) \end{aligned} \quad (7)$$

The average entropy production rate $\dot{\mathcal{S}}$ of the process (1) is obtained by taking the expectation value of (7) over $\dot{x}(t)$ and taking the limit as $T \rightarrow \infty$.

We expanded up to order ν^3 , but the contributions we find are smaller than this. We can do this because w , x , and V never appear alone in any term, but they always accompany each other at least in pairs. This means that the contribution from terms that are $\mathcal{O}(\nu^4)$ is at most $\mathcal{O}(\nu^8)$.

III. ASYMMETRIC RUN-AND-TUMBLE PROCESS

A. Description of the process

We will now specialise to the case where $V \equiv 0$ and $w(t)$ is an asymmetric, mean-zero telegraph process. In other words, the Langevin equation now reads

$$\dot{x} = \nu w(t) + \xi(t), \quad (8)$$

which describes an asymmetric RnT particle in one dimension. Note that in such a case we can easily deduce the n -th order autocorrelation function of \dot{x} from Eqn. 8. We have

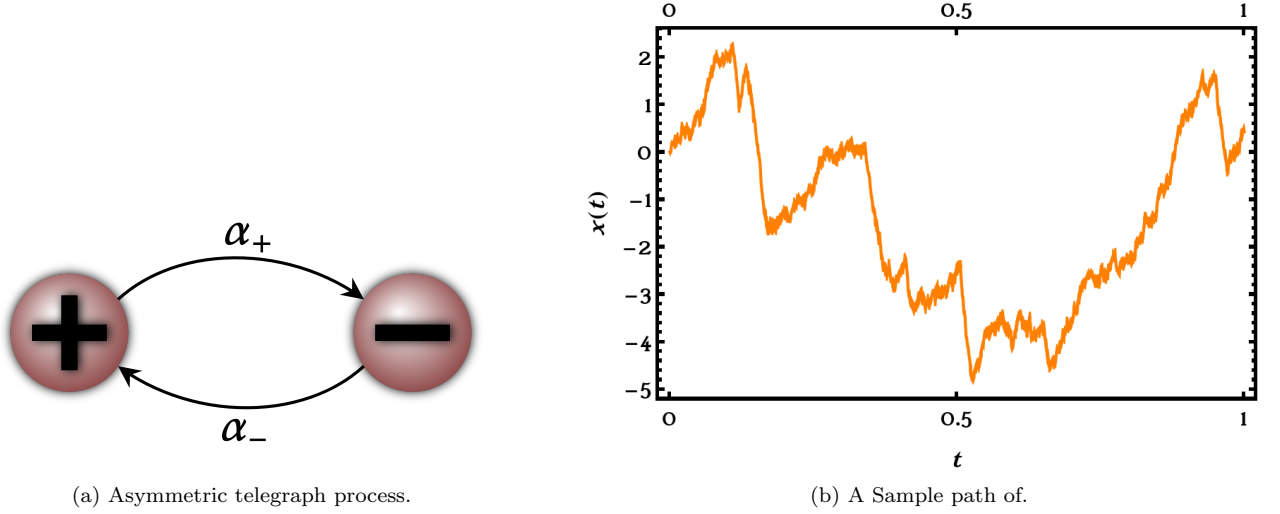


FIG. 1. 1a shows a diagram of the telegraph process $w(t)$ as discussed in Section III. In the +ve state, the particle has self-propulsion νw_+ , and in the -ve state the self-propulsion is νw_- . Since $\bar{w} = 0$, we have $\alpha_+ w_- + \alpha_- w_+ = 0$. 1b depicts a sample path for the particle governed by 2 where w is an asymmetric telegraph process with zero mean.

$$\langle \dot{x} \rangle = \nu \bar{w}, \quad (9)$$

$$\langle \dot{x}(t_1) \dot{x}(t_2) \rangle = \nu^2 \overline{w(t_1)w(t_2)} + 2D\delta(t_1 - t_2), \quad (10)$$

$$\langle \dot{x}(t_1) \dot{x}(t_2) \dot{x}(t_3) \rangle = \nu^3 \overline{w(t_1)w(t_2)w(t_3)}, \quad (11)$$

Hence, by Eqn. (7), the entropy production rate of such a process is

$$\begin{aligned} \dot{S} = & \frac{\nu^2}{TD} \int_0^T dt \left(\overline{w(t)} \right)^2 + \frac{\nu^4}{4TD^2} \int_0^T dt_1 dt_2 \left(\overline{w(t_1)} \right)^2 \cdot \overline{w(t_2)^2} + \frac{\nu^6}{T} \left[\frac{1}{24D^3} \int_0^T dt_1 dt_2 dt_3 \left(\overline{w(t_1)w(t_2)w(t_3)} \right)^2 \right. \\ & \left. - \frac{1}{8D^3} \int_0^T dt_1 dt_2 dt_3 \overline{w(t_1)} \cdot \overline{w(t_2)w(t_3)} \cdot \overline{w(t_1)w(t_2)w(t_3)} \right] + \mathcal{O}(\nu^8) \end{aligned} \quad (12)$$

The telegraph process $w(t)$ switches between two values w_+ and w_- , with rates α_+ and α_- . These values are constrained by the zero-mean condition

$$\overline{w(t)} = \frac{w_+ \alpha_- + w_- \alpha_+}{\alpha_+ + \alpha_-} = 0. \quad (13)$$

Whenever this zero-mean condition is satisfied, the leading order contribution in Eqn. (12) is given by

$$\boxed{\dot{S} = \frac{\nu^6}{24TD^3} \int_0^T dt_1 dt_2 dt_3 \left(\overline{w(t_1)w(t_2)w(t_3)} \right)^2} \quad (14)$$

In the subsequent section, the three-time correlation function (and thus the leading-order entropy production) is derived in closed form.

B. Calculation of three-time correlation function

The asymmetric Run-and-Tumble process is represented by the master equation

$$\frac{d}{dt} \begin{pmatrix} p_+(t) \\ p_-(t) \end{pmatrix} = \begin{pmatrix} -\alpha_+ & \alpha_- \\ \alpha_+ & -\alpha_- \end{pmatrix} \begin{pmatrix} p_+(t) \\ p_-(t) \end{pmatrix} \quad (15)$$

where $p_+(t)$ is the probability of the process $w(t)$ taking the value w_+ at time t and $p_-(t) = 1 - p_+(t)$ is the probability that $w(t)$ takes the value w_- . This is solved exactly with appropriate boundary conditions and produces the following matrix elements:

$$\begin{aligned} P_{++}(t) &= \frac{1}{\alpha_+ + \alpha_-} \left(\alpha_- + \alpha_+ e^{-(\alpha_+ + \alpha_-)t} \right) \\ P_{-+}(t) &= \frac{1}{\alpha_+ + \alpha_-} \left(\alpha_+ - \alpha_- e^{-(\alpha_+ + \alpha_-)t} \right) \\ P_{+-}(t) &= \frac{1}{\alpha_+ + \alpha_-} \left(\alpha_- - \alpha_+ e^{-(\alpha_+ + \alpha_-)t} \right) \\ P_{--}(t) &= \frac{1}{\alpha_+ + \alpha_-} \left(\alpha_+ + \alpha_- e^{-(\alpha_+ + \alpha_-)t} \right) \end{aligned} \quad (16)$$

where $P_{-+}(t)$ is the probability of $w(t)$ taking a value w_- having been initialised at $t = 0$ with value w_+ . The three-time correlation function of $w(t)$ is expressed as follows:

$$\begin{aligned} \overline{w(t_3)w(t_2)w(t_1)} &= \mathcal{I}(t_3 > t_2 > t_1) \begin{pmatrix} 1 & 1 \end{pmatrix} M_w(t_3 - t_2) M_w(t_2 - t_1) \begin{pmatrix} w_+ P_+ \\ w_- P_- \end{pmatrix} \\ &+ \mathcal{I}(t_2 > t_3 > t_1) \begin{pmatrix} 1 & 1 \end{pmatrix} M_w(t_2 - t_3) M_w(t_3 - t_1) \begin{pmatrix} w_+ P_+ \\ w_- P_- \end{pmatrix} + \dots \end{aligned} \quad (17)$$

where $P_{+/-} = \lim_{t \rightarrow \infty} P_{++/-}(t)$ are the stationary probabilities of $w(t)$ taking the value $w_{+/-}$ and $\mathcal{I}(t_3 > t_2 > t_1)$ are indicator functions which impose time-ordering. The transition matrices $M_w(t)$ are given by

$$M_w(t) = \begin{pmatrix} w_+ P_{++}(t) & w_+ P_{+-}(t) \\ w_- P_{-+}(t) & w_- P_{--}(t) \end{pmatrix} \quad (18)$$

The form of equations (16) allows the expression of the transition matrices $M_w(t)$ in the more convenient form

$$\begin{aligned} M_w(t) &= M_{w0} + M_{w1} e^{-(\alpha_+ + \alpha_-)t} \\ M_{w0} &= \frac{1}{\alpha_+ + \alpha_-} \begin{pmatrix} w_+ \alpha_- & w_+ \alpha_- \\ w_- \alpha_+ & w_- \alpha_+ \end{pmatrix} \\ M_{w1} &= \frac{1}{\alpha_+ + \alpha_-} \begin{pmatrix} w_+ \alpha_+ & -w_+ \alpha_- \\ -w_- \alpha_+ & w_- \alpha_- \end{pmatrix} \end{aligned} \quad (19)$$

Equation (17) is simplified by the following

$$\begin{pmatrix} 1 & 1 \end{pmatrix} M_{w0} = M_{w0} \begin{pmatrix} w_+ P_+ \\ w_- P_- \end{pmatrix} = 0 \quad (20)$$

so that the three-time correlation function is given by

$$\begin{aligned} \overline{w(t_3)w(t_2)w(t_1)} &= \begin{pmatrix} 1 & 1 \end{pmatrix} M_{w1}^2 \begin{pmatrix} w_+ P_+ \\ w_- P_- \end{pmatrix} e^{-(\alpha_+ + \alpha_-)(t_3 - t_1)} \\ &= \frac{\alpha_+ \alpha_- (\alpha_+ w_+ + \alpha_- w_-) (w_+ - w_-)^2}{(\alpha_+ + \alpha_-)^3} \left[e^{-(\alpha_+ + \alpha_-)(t_3 - t_1)} \mathcal{I}(t_3 > t_1) + e^{-(\alpha_+ + \alpha_-)(t_2 - t_1)} \mathcal{I}(t_2 > t_1) + \dots \right] \end{aligned} \quad (21)$$

Using this in equation (14) yields

$$\dot{S} = \frac{\nu^6}{4 \cdot 3! \cdot TD^3} \left[\frac{\alpha_+ \alpha_- (\alpha_+ w_+ + \alpha_- w_-) (w_+ - w_-)^2}{(\alpha_+ + \alpha_-)^3} \right]^2 \int_0^T dt_1 dt_2 dt_3 \left[e^{-(\alpha_+ + \alpha_-)(t_3 - t_1)} \mathcal{I}(t_3 > t_2 > t_1) \right. \\ \left. + e^{-(\alpha_+ + \alpha_-)(t_2 - t_1)} \mathcal{I}(t_2 > t_3 > t_1) + \dots \right]^2 \quad (22)$$

Relabelling indices and using the definition of the indicator function gives the following:

$$\dot{S} = \frac{\nu^6}{4 \cdot 3! \cdot TD^3} \left[\frac{\alpha_+ \alpha_- (\alpha_+ w_+ + \alpha_- w_-) (w_+ - w_-)^2}{(\alpha_+ + \alpha_-)^3} \right]^2 \cdot 6 \int_0^T dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 e^{-2(\alpha_+ + \alpha_-)(t_3 - t_1)} \\ = \frac{\nu^6}{16TD^3} \cdot \frac{\alpha_+^2 \alpha_-^2 (\alpha_+ w_+ + \alpha_- w_-)^2 (w_+ - w_-)^4}{(\alpha_+ + \alpha_-)^8} \quad (23)$$

Rearranging and using equation (13) produces the following expression:

$$\boxed{\dot{S} = -\frac{\nu^6}{16D^3} \cdot \frac{w_+^3 w_-^3}{\alpha_+ \alpha_-} \left(\frac{\alpha_+ - \alpha_-}{\alpha_+ + \alpha_-} \right)^2} \quad (24)$$

IV. EXTENSION TO CONFINED PARTICLES

We will consider now the case of the symmetric RnT particle confined in a harmonic potential of strength k . Accordingly, let $w(t)$ be a telegraph process as in Section III with parameters

$$\alpha_- = \alpha_+ =: \alpha, \quad -w_- = w_+ =: w_0, \quad (25)$$

and $V(x) = kx^2/2$. Note that if the potential V has no explicit time-dependence, we have

$$\frac{1}{D} \left\langle \int_0^T \dot{x} \frac{\partial V}{\partial x} dt \right\rangle = \frac{1}{D} \left\langle \int_0^T \left(\frac{dV}{dt} - \frac{\partial V}{\partial t} \right) dt \right\rangle \quad (26)$$

$$= \frac{1}{D} \left\langle \int_0^T \frac{dV}{dt} dt \right\rangle = \frac{1}{D} \left\langle V(x(t)) \Big|_0^T \right\rangle = 0. \quad (27)$$

Hence, the zeroth-order term in Eqn. (7) does not contribute to the entropy production. Therefore the leading order contribution to the entropy production rate of the particle is given by

$$\boxed{\dot{S} = -\frac{\nu^2 k}{2TD^2} \int_0^T dt_1 dt_2 \overline{\overline{w(t_1)w(t_2)}} \langle \dot{x}(t_1) x(t_2) \rangle}. \quad (28)$$

The autocorrelation $\overline{\overline{w(t_1)w(t_2)}}$ can be calculated using the same methods as in Section III to obtain

$$\overline{\overline{w(t_1)w(t_2)}} = w_0^2 e^{-2\alpha|t_2 - t_1|}. \quad (29)$$

Moreover, using Eqn. (2), we can write

$$\begin{aligned}\langle \dot{x}(t_1)x(t_2) \rangle &= \left\langle \left(\nu w(t_1) - kx(t_1) + \xi(t_1) \right) \cdot \left(\int_0^{t_2} ds (\nu w(s) - kx(s)) + B(t_2) \right) \right\rangle, \\ &= -k \langle x(t_1)B(t_2) \rangle + k^2 \int_0^{t_2} \langle x(t_1)x(s) \rangle ds - k \int_0^{t_2} \langle \xi(t_1)x(s) \rangle ds + \langle \xi(t_1)B(t_2) \rangle + \mathcal{O}(\nu)\end{aligned}\quad (30)$$

where $B(t)$ is a Brownian motion.

Can we make sense of this? I think so - use correlators from Rosalba to expand term-by-term.

V. DISCUSSION

In Section II we present a systematic perturbation framework for calculating the entropy production of self-propelling particles subject to a potential. In general, obtaining a closed form expression may be difficult when using this framework. However, in particular cases of interest, such as when the net current is zero or the potential considered is time-independent, the calculations simplify considerably, allowing us to obtain closed-form expressions for the leading order contributions to entropy production.

This is demonstrated in Sections III & IV. In Section III we derive the leading order contribution to the entropy production for a free asymmetric RnT particle. Using the zero-mean constraint given by Eqn. (13), we can rewrite the result from Eqn. (24) as

$$\dot{\mathcal{S}} = \frac{\nu^6}{16D^3} \frac{\bar{w}^6}{\bar{\alpha}^2} \left(\frac{1-\lambda}{1+\lambda} \right)^2, \quad (31)$$

where $\bar{w} = \sqrt{|w_+ w_-|}$ and $\bar{\alpha} = \sqrt{\alpha_+ \alpha_-}$ are the geometric average speed and transition rate respectively, and

$$\lambda := \left| \frac{w_-}{w_+} \right| = \frac{\alpha_-}{\alpha_+}. \quad (32)$$

Eqn. (31) illuminates the dependence of $\dot{\mathcal{S}}$ on the ratio of the speeds, λ . The entropy production disappears at $\lambda = 1$ as expected. For fixed values of \bar{w} and $\bar{\alpha}$ the maximum entropy production

$$\dot{\mathcal{S}}_{\max} = \frac{\nu^6}{16D^3} \frac{\bar{w}^6}{\bar{\alpha}^2} \quad (33)$$

is achieved in the limits as $\lambda \rightarrow 0$ and $\lambda \rightarrow \infty$. This is consistent with the principle that *something here about finite power producing finite entropy*. Moreover, in the strong diffusion regime where

$$D \gg \frac{\bar{w}^2}{\bar{\alpha}}, \quad (34)$$

the noise dominates the self-propulsion kinetics and the entropy production disappears. In other words, the entropy production becomes negligible whenever

$$\bar{\alpha} \gg \frac{\bar{w}^2}{D}. \quad (35)$$

The factor \bar{w}^2/D is analogous to the v^2/D term which appears in the entropy production of a diffusion process with constant self-propulsion speed v . When the condition in (35) is satisfied, the high transition rate effectively masks the self-propulsion of the particle, resulting in reduced entropy production.

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