Stochastic thermodynamics of active Brownian particles

Chandrima Ganguly\textsuperscript{1} and Debasish Chaudhuri\textsuperscript{1,\textdagger}

\textsuperscript{1}Indian Institute of Technology Hyderabad, Yeddumasilaram 502205, Andhra Pradesh, India

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Examples of self propulsion in strongly fluctuating environment is abound in nature, e.g., molecular motors and pumps operating in living cells. Starting from Langevin equation of motion, we develop a stochastic thermodynamic description of non-interacting self propelled particles using simple models of velocity dependent forces. We derive fluctuation theorems for entropy production and a modified fluctuation dissipation relation, characterizing the linear response at non-equilibrium steady states. We study these notions in a simple model of molecular motors, and in the Rayleigh-Helmholtz and energy-depot model of self propelled particles.

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I. INTRODUCTION

Living systems are by definition open and active, staying out of equilibrium by consuming and subsequently dissipating energy, thereby generating forces and motion. Subcellular components, e.g., motor proteins, cytoskeletal filaments etc. operate in a stochastic environment, where fluctuations arise from thermal motion and, in many cases, chemical reactions \textsuperscript{[1]}. In contrast to conventional Brownian motion where the forces acting on a particle are entirely due to external sources, the active Brownian particles can generate their own forces \textsuperscript{[2]} utilizing chemical energies \textsuperscript{[1]}.

Traditional thermodynamics in terms of average quantities does not provide satisfactory description of small assembly of colloidal particles, or nano-materials due to the presence of strong thermal fluctuations. In the last two decades, a theoretical framework has emerged that allows several exact relations for distributions of fluctuating quantities like work, heat and entropy characterizing individual trajectories of the particles \textsuperscript{[3–16]}. At non-equilibrium steady states (NESS) entropy $\sigma$ is continually produced, with its probability distribution obeying $P(\sigma)/P(-\sigma) = \exp(\sigma/k_B)$. This is known as the detailed fluctuation theorem (DFT) and was first observed in simulations of sheared liquids \textsuperscript{[16]} and later derived using chaotic \textsuperscript{[15]} and stochastic dynamics \textsuperscript{[10, 13]}. For asymptotic steady states the above relation is obeyed with $\sigma = \Delta s_m, \Delta s_m$ being the change in entropy of the medium alone. If one considers the stochastic change in system entropy $\Delta s$ as well, $\sigma = \Delta s_{tot} = \Delta s + \Delta s_m$ signifying the total entropy change, the DFT remains valid even for finite time measurements \textsuperscript{[17]}. Further, $\Delta s_{tot}$ obeys an integral fluctuation theorem $\exp(-\Delta s_{tot}/k_B) = 1$ where $\langle \ldots \rangle$ denotes non-equilibrium average over stochastic paths. This is closely related to the Jarzynski equation, that expresses equilibrium free energy difference in terms of non-equilibrium work done \textsuperscript{[12, 14]}.

These fluctuation theorems were verified in experiments on colloids \textsuperscript{[18–20]} and granular matter \textsuperscript{[21]}, and successfully used to find out the free energy landscape of RNA \textsuperscript{[22, 23]}. Fluctuation theorems were also derived for the flashing ratchet \textsuperscript{[24, 25]} and other detailed models of molecular motors and enzymes \textsuperscript{[26]}. However, given the complexity of living systems it may not always be possible to identify and model all the chemical processes and mechano-chemical coupling responsible for autonomous force generation. Recently, the DFT was applied to measure the torque generation by a rotary motor \textsuperscript{[27]} from its fluctuating trajectories \textsuperscript{[28]}. This idea may be extended to other types of molecular motors to measure autonomous force or torque generation from their stochastic trajectories \textsuperscript{[28]}.

Response in equilibrium states is characterized by the fluctuation-dissipation theorem (FDT), and the ratio of correlation and response is often interpreted as effective temperature of systems at NESS \textsuperscript{[29, 30]}. Recent theoretical work derived several forms of modified fluctuation-dissipation relations (MFDR) characterizing linear response at NESS and established additive correction to FDT due to the presence of non-zero steady state currents \textsuperscript{[31, 32]}, thus showing that phenomenological characterization of active processes by effective temperatures is not consistent. Some of the theoretical predictions were verified experimentally \textsuperscript{[33, 34]}.

In this paper, starting from the equation of motion for a self propelled particle (SPP) immersed in a Langevin heat bath, we develop its stochastic thermodynamic description. We assume that the self-propulsion force is velocity dependent, however, the details of the propulsion mechanism is not specified to begin with. Using this assumption, we derive energy balance relation and fluctuation theorems involving entropy production. In particular, we identify the contributions in entropy production due to self-propulsion and its coupling to external drive. We also obtain a modified fluctuation-dissipation relation characterising the linear response at steady states of an SPP. Finally, we use our theoretical development to study some specific model systems that utilises velocity dependent forces: a simple model of molecular motors obeying a linear force-velocity relation, and models utili-
ising non-linear velocity dependent forces as self propulsion mechanism, namely, the Rayleigh-Helmholtz model and the energy-depot model.

II. LANGEVIN EQUATION AND THE LAWS OF THERMODYNAMICS

To develop the notions of stochastic thermodynamics of SPP systems, let us focus on one dimension (1d), for simplicity. Simplest models of SPPs, like that the Rayleigh-Helmholtz model or the energy-depot model, use velocity dependent autonomous force \( F(v) \) to model self-propulsion. The Langevin equation for the motion of each particle evolving in the presence of a time dependent external force \( f(t) \) has the form

\[
\begin{align*}
\dot{x} &= v \\
\dot{v} &= -\gamma v + \eta + F(v) - \frac{\partial U(x)}{\partial x} + f(t)
\end{align*}
\]  

(1)

where \(-\gamma v\) is viscous dissipation, \( \eta \) is Gaussian white noise characterized by \( \langle \eta(t) \rangle = 0, \langle \eta(t) \eta(t') \rangle = 2D_0 \delta(t - t') \) with \( D_0 = \gamma k_B T \), \( U(x) \) is a conservative external potential. We use particle mass \( m = 1 \), unless otherwise specified.

A. First law

Multiplying the above equation by velocity \( v \) and integrating over a small time interval \( \tau \) one obtains the first law [40]

\[
\Delta E = \Delta W + \Delta q
\]

(2)

where \( E = (1/2)v^2 + U(x) \), \( \Delta E \) denoting the change in internal energy, \( \Delta W = \int_0^\tau dt \, v \cdot f(t) \) the work done on the SPP by external force, and the total heat flow \( \Delta q = \Delta Q + \Delta Q_m \) has two components, \( \Delta Q = \int_0^\tau dt \, v \cdot (-\gamma v + \eta) \) the energy flow from the heat bath, \( \Delta Q_m = \int_0^\tau dt \, v \cdot F(v) \) the energy flow from the internal motor degrees of freedom of the SPP. The presence of energy flow from internal motor differentiates SPPs from passive Brownian particles [41].

B. Fluctuation theorem: connection with second law

Consider the time evolution of the system from \( t = 0 \) to \( \tau \) through a path defined by \( X = \{x(t), v(t), f(t)\} \). The probability of this path is given by (see Appendix-A)

\[
\begin{align*}
\mathcal{P}_+ &= \mathcal{N} \delta(\dot{x} - v) \exp \left[ -\frac{1}{2} \int_0^\tau dt \frac{\partial g(v)}{\partial v} \right] \\
&\times \exp \left[ -\frac{1}{4D_0} \int_0^\tau dt \left( \dot{v} - g(v) + \frac{\partial U}{\partial x} - f(t) \right)^2 \right]
\end{align*}
\]  

(3)

where \( \mathcal{N} \) is a normalisation constant. We used the symbol \( g(v) = -\gamma v + F(v) \) for brevity. Reversing the velocities gives us the time reversed path \( X^\dagger = \{x'(t'), v'(t'), f'(t')\} = \{x(\tau - t), -v(\tau - t), f(\tau - t)\} \), the probability of which can be expressed as

\[
\begin{align*}
\mathcal{P}_- &= \mathcal{N} \delta(\dot{x} - v) \exp \left[ -\frac{1}{2} \int_0^\tau dt \frac{\partial g(v)}{\partial v} \right] \\
&\times \exp \left[ -\frac{1}{4D_0} \int_0^\tau dt \left( \dot{v} + g(v) + \frac{\partial U}{\partial x} - f(t) \right)^2 \right]
\end{align*}
\]  

(4)

where in the last step it was assumed that \( g(v) \) is an odd function \( g(-v) = -g(v) \). This condition is naturally satisfied in many SPP models that assume energy transduction from internal energy source to kinetic energy [42], as will be illustrated further in the following sections. Thus the ratio of the probabilities of the forward and reverse paths comes out to be

\[
\frac{\mathcal{P}_+}{\mathcal{P}_-} = \exp \left[ -\beta \left( \Delta q + \Delta Q_{em} + \frac{1}{\gamma} \Delta \phi \right) \right]
\]

(5)

where \( \beta = 1/k_B T = \gamma / D_0 \). In the above relation \( \Delta q \) is the heat flow identified in the first law. The term \( \Delta Q_{em} = (1/\gamma) \int_0^\tau dt \, F(v).\dot{f}(t) - \partial U \) is due to the coupling between the internal motor degrees of freedom and mechanical forces, \( \Delta \phi \) is the change in a velocity dependent potential defined through \( F(v) = -\partial \phi(v) / \partial v \).

Eq. (5) gives the ratio of the probabilities of forward and reverse paths, given that the forward evolution takes the system from initial state \( o \) to final state \( e \). Assuming that the normalized probability distribution of these two states are \( \pi_o \) and \( \pi_e \), respectively, the ratio of the forward and the reverse processes is

\[
\frac{P_f(X)}{P_r(X)} = \frac{\pi_o \mathcal{P}_+}{\pi_e \mathcal{P}_-} = e^{\Delta s / k_B} e^{-\beta \left( \Delta q + \Delta Q_{em} + \frac{1}{\gamma} \Delta \phi \right)} = \exp[\Delta s_f / k_B]
\]

(6)

where we used the stochastic entropy content corresponding to the distributions of initial and final states given by \( s_{o,e} = -k_B \ln \pi_{o,e} \) [17], leading to \( \pi_o / \pi_e = \exp(\Delta s_f / k_B) \). The total entropy production in the forward process is

\[
\Delta s_f = \Delta s - \frac{1}{T} \left( \Delta q + \Delta Q_{em} + \frac{1}{\gamma} \Delta \phi \right)
\]

(7)

where in the last step we used Eq. (2).

The main contribution of this paper is the identification of this total entropy production Eq. (7), which contains two new terms as compared to a system of traditional Brownian particles. These are the energy exchange
between the motor’s internal degrees of freedom and the external mechanical forces $\Delta Q_{em}$, and a change in the velocity dependent potential $\Delta \phi$. Both these contributions disappear once the motor activity of the self-propelled particles is switched off. Note that both $\Delta Q_{em}$ and $\Delta \phi(v)$ are hidden from the perspective of the first law, but appears in the expression of the total entropy change. This is due to the intrinsic open nature of the system with respect to the self propulsion mechanism.

Eq. (10) implies the integral fluctuation theorem \[ \langle e^{-\Delta s_t/k_B} \rangle = \int D[X] \frac{P_r(X)}{P_f(X)} \frac{P_f(X)}{P_r(X)} = \int D[X] P_r(X) = 1. \] (8)

This leads to $\langle \Delta s_t \rangle \geq 0$, a positive average entropy production. Note that Eq. (8) together with Eq. (7) gives $\langle e^{-\beta \Delta W} \rangle = \langle e^{- \beta (\Delta E - T \Delta s_t)} \rangle \text{ where } \Delta A = \Delta E - T \Delta s_t$. In the absence of motor driving, $\Delta Q_{em} = 0$ and $\Delta \phi = 0$, $\Delta A$ is in Helmholtz free energy, and the above relation gives the Jarzynski equation $\langle \exp(-\beta \Delta W) \rangle = \exp(-\beta \Delta A) \tag{14}$

C. Stochastic thermodynamics at NESS

It can be shown that at NESS the detailed fluctuation theorem (see Appendix C) holds, where $\Delta s_t$ is the total entropy change along any trajectory.

Calculation of total entropy takes a simple form when $U(x) = 0$. We derive this result here, as it will be used in the context of particular models of velocity dependent force in later sections. The Langevin equation in presence of a constant external force is $\dot{v} = - \dot{\psi}(v)/\dot{v} + \eta$, with $\dot{\psi}(v)/\dot{v} = -\gamma v + F(v) + f$. The corresponding Fokker-Planck equation has the form $\partial_v p(v,t) = D_0 \partial_v \left[ -\psi(D_0 \partial_v \psi(v)/D_0 p) \right]$ with a steady state solution $p_s(v) = \frac{1}{Z} e^{-\psi(v)/D_0} \tag{10}$

where the normalization $Z = \int_{-\infty}^{\infty} dv \exp(-\psi(v)/D_0)$, and $\psi(v) = (\gamma v^2/2 - f v) + \phi(v)$ with $\phi(v) = -\int dv F(v)$, as before. At NESS entropy is continually produced, and the system entropy change is $\Delta s_t/k_B = \Delta \psi/D_0$. Thus the total entropy production $\langle \Delta s_t \rangle$ is

$$\frac{\Delta s_t}{k_B} = \beta \left( -\frac{1}{\gamma} f \Delta \psi + \Delta W - \Delta Q_{em} \right), \tag{11}$$

where $-f \Delta \psi/\gamma$ denotes work done by the SPP due to its change in velocity. The energy flux $\Delta Q_{em}$, and work done $\Delta W$ have the same meaning as discussed in the previous subsection. The total entropy production in NESS obeys both the integral and detailed fluctuation theorems of Eqs (3) and (9).

III. LINEAR RESPONSE AT NESS: MODIFIED FLUCTUATION DISSIPATION RELATION

The Fokker-Planck equation corresponding to Eq. (11) is $\partial_t p(x,v,t) = L(x,v,h) p(x,v,t) = (L_0 + f(t) L_1) p \tag{12}$

where

$$L_0 p = -\partial_x [g(v) - \partial_x U] p + D_0 \partial_v^2 p \tag{13}$$

$$L_1 p = -\partial_v p. \tag{14}$$

Assuming that the SPP system goes to a steady state characterized by a distribution function $p_s$ obeying $L_0 p_s = 0$, linear response around this steady state is described by $35 \ 37 \ \ 38$

$$\frac{\delta \langle A(t) \rangle}{\delta f(t')} = \frac{1}{D_0} \langle A(t)[\gamma v(t') - F(v(t'))] \rangle_s = \beta \langle A(t)v(t') \rangle_s - \frac{1}{D_0} \langle A(t)F(v(t')) \rangle_s. \tag{15}$$

This is the modified fluctuation dissipation relation (MFDR) characterizing response function at NESS of SPP. In the absence of self propulsion, $F(v) = 0$, one gets back the equilibrium fluctuation dissipation theorem (FDT). The velocity response to external force is

$$\chi(t,t') = \frac{\delta \langle v(t) \rangle}{\delta f(t')} = \beta \langle v(t)v(t') \rangle_s - \frac{1}{D_0} \langle v(t)F(v(t')) \rangle_s. \tag{15}$$

Since the correction in MFDR at NESS with respect to the equilibrium FDT is additive (see Eq. (15), not multiplicative, a ratio of the correlation and response $\langle v(t)v(t') \rangle/\chi(t,t')$ can not, in general, be interpreted as an effective temperature, with the only possible exception being when $F(v)$ is a linear function of velocity $v$.

In the following, we consider some specific models of self propelled particles and analyze their behavior using the formalism developed so far.

IV. MODELS OF SPP

In this section we consider three specific examples of SPP. The first one is the simplest, uses a linear force-velocity relation that sometimes is used to describe Kinesin like motor proteins\[14]. The second and
third example use non-linear velocity-dependent forces. The second example deals with the Rayleigh-Helmholtz model\cite{12} which has been useful to describe the collective motion of a bunch of motor proteins working in tandem to move appropriate cargo\cite{13}. In the third example we use the energy-depot model \cite{42, 46}, which utilizes a simple coupling between internal energy production and mechanical motion to propel particles.

A. Molecular motors

Molecular motors, e.g., kinesins move on polymeric tracks, e.g., microtubules in a highly stochastic but directed manner utilizing chemical energy from ATP hydrolysis. In the presence of load force acting in the direction opposing their motion, they slow down and eventually stop moving. This behavior can be approximately modeled through a linear force-velocity relation \cite{17}. Let us assume the autonomous force produced by the motor is $f_s$. In the presence of an external load force $-\lambda$, the Langevin equation is

$$\dot{v} = -\gamma v + \eta + f_s - \lambda.$$  \hspace{2cm} (16)

In the over-damped limit, this leads to the linear force-velocity relation $\langle v \rangle = v_0(1 - \lambda/f_s)$ with $v_0 = f_s/\gamma$ the autonomous velocity of free motors, and $f_s$ the stall force. Note that, using a linear velocity dependent force $f_s(1 - v/v_0)$ in place of $f_s$, merely changes the effective viscous drag $\gamma$ in the above equation by a constant additive amount. In molecular motors, the mechano-chemical processes leading to self propulsion, in general, may elevate the noise level, change the noise correlation, and change the viscous drag. However, in this simple model we assume that the noise can still be regarded as white if the time resolution is not too small, and the effective diffusion constant contains the impact of chemical reactions. In the absence of external load $\lambda = 0$, the Langevin equation can be rewritten as $\dot{v} = -\psi'(v) + \eta$ where $\psi'(v) \equiv \partial \psi / \partial v = \gamma v - f_s$ is obtainable from $\psi(v) = (\gamma/2)(v-v_0)^2$. Thus the steady state distribution (Eq.\textsuperscript{10})

$$p_s(v) = \sqrt{\frac{\beta}{2\pi}} \exp \left( -\frac{\beta}{2}(v-v_0)^2 \right).$$  \hspace{2cm} (17)

1. Entropy production at NESS

The total entropy production can be obtained from Eq.\textsuperscript{11}. Combining the constant self propulsion force $f_s$ with the load force $-\lambda$, the terms in Eq.\textsuperscript{11} $f = f_s - \lambda$, $F(v) = 0$, $\Delta Q_{em} = 0$ gives the total stochastic entropy production

$$\frac{\Delta s_t}{k_B} = \beta \left[ -\frac{1}{\gamma}(f_s - \lambda) \Delta v + \Delta W \right],$$  \hspace{2cm} (18)

with $\Delta W = (f_s - \lambda) \int_0^T v dt$. The integral and the detailed fluctuation theorems will be obeyed by this total entropy production at steady state.

One can extend this calculation to rotating motors, by replacing linear displacements by rotation, velocities by angular velocities, and forces by torques. Note that for measurements over asymptotically long time $\tau$, $\Delta W$ in the above expression becomes predominant and hence $\Delta s_t/k_B = \beta \Delta W$, the form used in recent experiments on $\text{F}_1\text{ATPase}$ \cite{27}.

2. Entropy production at oscillatory steady states

In the presence of a time-dependent external force the Langevin equation describing the molecular motor is

$$\dot{v} = -\gamma v + \eta + f_s + f(t),$$  \hspace{2cm} (19)

where $\langle v(t) \rangle = v_0 + \int_0^t dt' e^{-\gamma(t-t')} [f(t') + \eta(t')]$. Thus $v(t)$ is a linear functional of Gaussian noise $\eta(t')$, implying that the probability distribution of $v(t)$ is also Gaussian,

$$p(v,t) = \sqrt{\frac{\beta}{2\pi}} \exp \left( -\frac{\beta}{2}(v - \langle v(t) \rangle)^2 \right)$$  \hspace{2cm} (20)

The system entropy production during a time $\tau$ is $\Delta s_t/k_B = -\ln[p(v(\tau), \tau)/p(v_0, 0)] = \beta(\bar{v} - \langle \bar{v} \rangle)(\Delta v - \langle \Delta v \rangle)$ with $\bar{v} = (v_T + v_0)/2$ and $\Delta v = v_T - v_0$. Thus the total entropy production is given by

$$\frac{\Delta s_t}{k_B} = \beta \Delta W - \langle \bar{v} \rangle \Delta v - \langle \bar{v} - \langle \bar{v} \rangle \rangle \Delta v.$$  \hspace{2cm} (21)

3. Linear response at NESS

It is straightforward to obtain the velocity response to a perturbing force around a steady state of free molecular motors using Eq.\textsuperscript{15}. $k_B T \delta \langle v(t) \rangle/\delta f(t') = \langle v(t) v(t') \rangle_s - v_0^2$. Using Eq.\textsuperscript{10} one can directly calculate the two-time correlation function $\langle v(t) v(t') \rangle_s = v_0^2 + k_B T e^{-\gamma|t-t'|}$. Thus one obtains the equilibrium-like response function

$$\frac{\delta \langle v(t) \rangle}{\delta f(t')} = e^{-\gamma|t-t'|}.$$  \hspace{2cm} (22)

In higher dimension, SPPs with a constant magnitude of self propulsion force $f_s$ can steer the direction of propulsion \cite{12}. Thus the impact of this force on the motion of SPP is different from an externally applied force
which is constant both in magnitude and direction. However, in 1d this difference disappears within the model described by Eq. (10). Steering the direction of self propulsion in 1d would mean switching the direction of motion from forward to backward. This is achieved in the following examples through non-linear velocity dependent self propulsion forces.

B. The Rayleigh-Helmholtz model

In the Rayleigh-Helmholtz (RH) model one assumes a non-linear velocity dependent force $F(v) = av - bv^3$. This is sometimes interpreted as a viscous force $F(v) = -\gamma_1(v)v$ with a viscosity $\gamma_1(v) = -a + bv^2$ where $-a$ acts like a negative friction that pumps energy into the system. In the deterministic limit, this model has two fixed points at $v = \pm \sqrt{a/b}$. In presence of a Langevin heat bath characterised by a viscous drag $\gamma$, the SPPs within RH model will experience a net negative drag $\gamma' = \gamma - a$ if $a > \gamma$, and the stochastic noise can switch the particles between positive and negative velocities $\pm \sqrt{(a - \gamma)/b}$. The RH model has recently been used in various studies of SPPs, and describes the bimodal velocity distribution of microtubules under the collective influence of bidirectional motor proteins NK11 [43].

1. Entropy production at NESS

In the presence of a constant external force $f$, one can write the total deterministic force as $-\psi'(v) = -\gamma v + F(v) + f$ such that $\psi(v) = (\gamma/2)v^2 - (a/2)(v - vf)^2 + (b/4)v^4$ with $vf = (f/a)$. Thus, using Eq. (10) one can find the steady state distribution

$$p_s(v, f) = \frac{1}{Z} \exp \left[-\beta \left(\frac{v^2}{2} - \frac{\alpha}{2}(v - vf)^2 + \frac{\nu}{4}v^4\right)\right] \tag{24}$$

where $\alpha = a/\gamma$ and $\nu = b/\gamma$. The corresponding stochastic entropy content is $s = -k_B \ln p_s$. It is straightforward to use Eq. (11) to obtain the total entropy production within a NESS. In a transformation from an initial state $p_s(v_0, f)$ to a final state $p_s(v, f)$,

$$\frac{\Delta s}{k_B} = \beta \left[-\alpha vf \left(vr - \frac{vf}{2}\right) - (\alpha - 1)\Delta W + \Delta W_0\right] \tag{25}$$

where $\Delta W = f \int^\tau vdt$ and $\Delta W_0 = \nu \int^\tau v^3dt$ grow with time $\tau$ and are the asymptotically dominant terms.

2. Linear response at NESS

The modified fluctuation dissipation relation, in this case, has the form

$$\chi(t, t') = \beta \langle v(t) v(t') \rangle_s - \frac{1}{T_0} \langle v(t)[av(t') - bv^3(t')] \rangle_s$$

$$= -\beta (\alpha - 1) \langle v^3(t') \rangle_s + \beta \nu \langle v(t) v^3(t') \rangle_s \tag{26}$$

Note that at $\alpha = 0 = \nu$ we have equilibrium, and obtain a fluctuation dissipation ratio $\langle v(t) v(t') \rangle_s/\chi(t, t') = k_B T$. However, in general this ratio depends on higher order correlations, and therefore on other quantities characterising a steady state.

3. Entropy production: external harmonic trap

If an initially free SPP is subjected to an external harmonic potential $\frac{1}{2}kx^2$, the initial steady state described by Eq. (24) undergoes transformation to a final steady state achieved in the trapping potential. The Langevin equation describing the dynamics of the SPP in trap is,

$$\dot{v} = -\gamma v + \eta(t) + F(v) - kx.$$  

The harmonic trap couples the time evolution of velocity with position. Multiplying the above equation by $v$ we get a Langevin equation for the time evolution of the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$, and $g(v) = -\gamma v + F(v) \tag{25}$ as before. In the deterministic limit of $\eta = 0$, the motion goes to fixed points governed by $g(v) = 0 \tag{25}$ at $v = \pm v_0$ with $v_0 = \sqrt{(a - \gamma)/b}$. This dynamics is characterised by $x = x_0 \sin(\omega t + \phi)$, $v = v_0 \cos(\omega t + \phi)$ with $\omega^2 = k$ and $x_0 = v_0/\omega$. The corresponding energy near these fixed points is $H \simeq H_0 = v^2_0$. The stochastic dynamics around these fixed points is described by the following Langevin equation

$$\frac{dH}{dt} = -\gamma H + \frac{dv}{dt}$$

has the steady state solution

$$p_s(H) = A \exp \left[-\frac{1}{D_0} \int \gamma_H dH\right].$$

The most probable energy is given by the fixed point $H = \frac{1}{2}v^2_0 + \frac{1}{2}kx^2 = H_0$ where $\gamma_H(H_0) = 0$. Thus near $H = H_0$ we can expand $\gamma_H$ as $\gamma_H = \beta(H - H_0)$ to obtain

$$p_s(H) = A \exp \left[-\frac{H}{2D_0} (H - H_0)^2\right]$$

which is equivalent to

$$\tilde{p}_s(x, v) = B e^{-\frac{1}{2\Delta^2} (x - H_0)^2} e^{-\frac{\beta}{2\nu_0^2} (\frac{x}{\Delta^2} - H_0)^2}\tag{27}$$

Note that the term $\exp[(-\beta \nu_0^2/2)x^2] \Delta^2$ implies that the particles with higher kinetic energies tend to locate near the potential minimum.
We now determine the change in entropy as the initial steady state characterized by $p_a(v_i,0)$ (Eq 24) is transformed to $\tilde{p}_a(x,v_f)$ given by Eq. (27). The change in system entropy is $\Delta s/k_B = -\ln[\tilde{p}_a(x,v_f) / p_a(v_i,0)]$, and the total entropy production in a trajectory (Eq.7),

$$\frac{\Delta s}{k_B} = \frac{\beta}{2} \left[ \frac{\nu}{4} (\omega^4 x^4) - (\alpha - 1) \omega^2 x^2 + \nu \omega^2 x^2 v_f^2 \right] - \beta[(\alpha - 1)\Delta W - \Delta W_0]$$

follows the integral and detailed fluctuation theorems given by Eq.s (8) and (9).

C. The energy depot model

Within the energy depot model (10), an SPP is capable of taking up external energy and store it in the internal energy depot, then transduce the energy into kinetic energy. A part of the stored energy is dissipated during conversion into kinetic energy. Thus the energy balance equation for an internal energy $e(t)$ is $de(t)/dt = q(r) - ce(t) - h(v)e(t)$ where $q(r)$ is the space dependent rate of energy uptake, and $h(v)$ is the rate of conversion of internal energy to kinetic energy. In a particular simple version of the model, one makes the choice $q(r) = q_0$, i.e., uniform energy uptake and $h(v) = dv^2$, conversion rate proportional to the kinetic energy itself. Assuming that $e(t)$ reaches its steady state value at a much shorter time scale than the particle diffusion time, we use its steady state value $e_0 = \frac{q_0}{c + dv^2}$. Then the self propulsion force is given by,

$$F(v) = ae_0v = \frac{aq_0v}{c + dv^2}. \quad (29)$$

In the limit of small velocities this model reduces to the Rayleigh-Helmholtz model $F(v) = \gamma_1 v - \gamma_2 v^3$ where $\gamma_1 = aq_0/c$ and $\gamma_2 = aq_0d/c^2$. Writing the total deterministic force acting on the SPP $-\omega^2 v - f(v) + ag_0/c + dv^2$, one gets $\psi(v) = \frac{q_0}{c + dv^2}$, conversion rate proportional to the kinetic energy itself. Thus using Eq. (10) the steady state distribution is

$$p_s(v,f) = \frac{1}{Z} (c + dv^2)^{aq_0/2Dd} e^{-\frac{\psi v^2}{2} + \frac{f^2}{4c}}. \quad (30)$$

The steady state entropy production due to a transformation from initial state $p_s(v_0,f)$ to a final state $p_s(v_f,f)$ is given by Eq. (11) with $\Delta W = f \int dt \eta$ and $\Delta Q_{em} = \int dt \eta v + v_0$ and $\Delta Q_{em} = (f/\gamma_1) \int dt \psi (c + dv^2)$. The linear response around $f = 0$ steady state can be expressed in terms of the modified fluctuation dissipation relation Eq. (15) with $F(v)$ given by Eq. (29), leading to

$$\chi(t,t') = \beta(\psi(t)\psi(t')) - \frac{aq_0}{D_0} \left( \frac{v(t')}{v(t)} \right). \quad (31)$$

V. CONCLUSION

We have presented a stochastic thermodynamic description of non-interacting self propelled particles in terms of energy conservation and fluctuation theorem. This enabled us to identify the components of stochastic entropy production associated with non-equilibrium processes in SPPs. We studied entropy production for a simple model of molecular motors, the Rayleigh-Helmholtz model, and the energy depot model. Calculation of entropy production and fluctuation theorems in SPPs has become important in view of recent experimental interest in measurement of force generation by molecular motors using the detailed fluctuation theorem (27, 28).

We further characterized the steady state response function in terms of a modified fluctuation-dissipation relation. This in general has an additive correction due to self propulsion, compared to the fluctuation-dissipation theorem at equilibrium. Our predictions for the Rayleigh-Helmholtz model are particularly amenable to experimental verification, due to its close relation to the motion of microtubules under collective influence of molecular motors NK11 [47, 53].

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Appendix A: Forward path probability

The probability of forward process is governed by the distribution of noise $\eta$ over time $\tau$ [11]

$$P[\eta] = N e^{-\frac{1}{2\sigma^2} \int_0^\tau dt \eta^2(t)} \quad (A1)$$

in presence of constraints $\dot{v} = g(v) - \partial U/\partial x + f(t) + \eta(t)$ and $x = v$. With paths denoted by $X = \{x(t), v(t), f(t)\}$, the forward path probability $P[X] = J P[\eta]$ where the Jacobian $J = det M$ and the Jacobi operator

$$M = \frac{\partial \eta}{\partial v} = \frac{\partial g(v)}{\partial v}. \quad (A2)$$

The Jacobian can be written as [53]

$$J = \exp[\text{Tr}(\ln M)] = \exp \left[ -\frac{1}{2} \int_0^\tau dt \frac{\partial g}{\partial v} \right] \quad (A3)$$

where in obtaining the last step, we discretised $M$ and used Stratonovich convention (see Appendix-A of Ref.[54]).

The discretisation process can be made explicit as follows. The time evolution of velocity can be discretised using the Stratonovich mid-point rule

$$\frac{v_i - v_i-1}{\epsilon} = \frac{1}{2} \left[ g_i(v_i) + g_i-1(v_i-1) \right] - \frac{1}{2} \left[ \frac{\partial U}{\partial x_i} + \frac{\partial U}{\partial x_{i-1}} \right]$$

$$+ \frac{1}{2} [f_i + f_{i-1}] + \eta_i \quad (A4)$$
where \( \langle \eta_i \rangle = 0 \) and \( \langle \eta_i \eta_j \rangle = 2(D_0/\epsilon)\delta_{ij} \) with total time \( \tau = N\epsilon \) discretised in \( N \) equal steps of size \( \epsilon \). Thus in the discretised notation the \( ik \)-th element of the \( N \times N \) Jacobi matrix \( M \) is

\[
M_{ik} = \frac{\partial \eta_i}{\partial v_k} = \frac{1}{\epsilon}(\delta_{i,k} - \delta_{i-1,k}) - \frac{1}{2}[g'_i(v_i)\delta_{i,k} + g'_{i-1}(v_{i-1})\delta_{i-1,k}]
\]  

(A5)

where \( g'_i(v_i) = \partial g_i(v_i)/\partial v_i \). Evaluating the determinant of this matrix one finds the Jacobian

\[
J = \det M = \left( \frac{1}{\epsilon} \right)^N \prod_{i=1}^{N} (1 - \frac{\epsilon}{2} g'_i(v_i))
\]

= \left( \frac{1}{\epsilon} \right)^N \exp \left[ \sum_{i=1}^{N} \ln \left( 1 - \frac{\epsilon}{2} g'_i(v_i) \right) \right]

\approx \left( \frac{1}{\epsilon} \right)^N \exp \left[ -\sum_{i=1}^{N} \frac{\epsilon}{2} g'_i(v_i) \right] \quad \text{(A6)}

Apart from a multiplicative constant, the Jacobian in the continuum limit can be expressed as,

\[
J = \exp \left[ -\frac{1}{2} \int_0^\tau dt \frac{\partial g}{\partial v} \right]. \quad \text{(A7)}
\]

Using the constraints of equations of motion, thus, one can obtain the probability of forward path \( [3] \)

\[
\mathcal{P}_+ = \delta(\dot{x} - v)N e^{-\frac{1}{k_B T} \int_0^\tau dt (-g(v) + \frac{\partial U}{\partial x} - f(v))} e^{-\frac{1}{2} \int_0^\tau dt \frac{\partial g}{\partial v}} \quad \text{(A8)}
\]

**Appendix B: Ratio of probabilities**

The ratio of the probabilities of the forward and reverse paths comes out to be

\[
\frac{\mathcal{P}_+}{\mathcal{P}_-} = \exp \left[ \frac{1}{D_0} \int_0^\tau dt \left( \dot{v} + \frac{\partial U}{\partial x} - f(t) \right) g(v) \right] = \exp \left[ \frac{1}{D_0} \int_0^\tau dt (-\gamma v + \eta + F(v))(-\gamma v + F(v)) \right] \quad \text{(B1)}
\]

where in the last step we used the Langevin equation and the expression of \( g(v) \). The terms in the exponential can be rewritten in the form

\[
\int_0^\tau dt (-\gamma v + \eta)(-\gamma v) + F(v)(F(v) - 2\gamma v + \eta) = -\gamma \Delta Q + \mathcal{I}
\]

(B2)

where the definition of \( \Delta Q \) is used from the first law Eq. (2), with the second term

\[
\mathcal{I} = \int_0^\tau dt \int_0^\tau df(v)\left[ \dot{\gamma} + \gamma v + F(v) \right] - f(t) - \partial_x U) \quad \text{(B3)}
\]

In the first term in the expression of \( \mathcal{I} \), we have used \( F(v) = -\partial \phi(v)/\partial v \) and thus \( \int_0^\tau dv \dot{\gamma} \dot{\phi}(v) = \phi(v(t)) - \phi(s, 0) = \Delta \phi \), the change in velocity dependent potential. The second term \( \Delta Q_m = \int_0^\tau dt F(v)(f(t) - \partial_x U) \). Thus we get the ratio in Eq. (4).

**Appendix C: Detailed fluctuation theorem**

It follows from Eq. (8) that the probability distribution of entropy production [10, 12]

\[
\rho(\Delta s_t) = \int \mathcal{D}[X] P_f(X) \delta(\Delta s_t - \Delta s_f(X))
\]

\[
= \int \mathcal{D}[X] P_r(X^\dagger) e^{-\Delta s_f/k_B} \delta(\Delta s_t - \Delta s_f(X))
\]

\[
= e^{\Delta s_t/k_B} \int \mathcal{D}[X^\dagger] P_r(X^\dagger) \delta(\Delta s_t + \Delta s_r(X^\dagger))
\]

\[
= e^{\Delta s_t/k_B} \rho(-\Delta s_t) \quad \text{(C1)}
\]

where we used \( \Delta s_f(X) = -\Delta s_r(X^\dagger) \), i.e., the final distribution of the forward process is assumed to be the same as the initial distribution of the reverse process, and vice versa [12]. This assumption is valid at steady states.

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