Entropy production of active particles formulated for underdamped dynamics

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The present work investigates the effect of inertia on the entropy production rate $\Pi$ for all canonical models of active particles for different dimensions and the type of confinement. To calculate $\Pi$, the link between the entropy production and dissipation of heat rate is explored resulting in a simple and intuitive expression. By analyzing the Kramers equation, alternative formulations of $\Pi$ are obtained and the virial theorem for active particles is derived. Exact results are obtained for particles in an unconfined environment and in a harmonic trap. In both cases, $\Pi$ is independent of temperature. For the case of a harmonic trap, $\Pi$ attains a maximal value for $\tau = \omega^{-1}$ where $\tau$ is the persistence time and $\omega$ is the natural frequency of an oscillator. For active particles in 1D box, or other non-harmonic potentials, thermal fluctuations are found to reduce $\Pi$.

I. INTRODUCTION

In this work we study the entropy production rate $\Pi$ [1–11] within underdamped dynamics for three canonical models of active particles. Contributions of inertia are expected to play role in the regime where the persistence time of active motion $\tau$ is comparable to or smaller than the inertial relaxation time $\tau_\text{r}$. Even if this regime may be inaccessible to experimental systems, the inclusion of inertia is necessary to recover a correct behavior in the limit $\tau \to 0$. Our interest to understand the role of inertia is motivated by a recently made observation that for the run-and-tumble (RTP) active Brownian particle (ABP) models the entropy production rate formulated within overdamped dynamics is maximal when $\tau = 0$ (implying a maximal distance from equilibrium) [12]. At the same time, the stationary distribution recovers a Boltzmann functional form (indicative of equilibrium) [12]. The present work shows that this inconsistency of conclusions is eliminated if $\Pi$ is defined in the underdamped dynamic regime, where as a result of inertia $\Pi$ vanishes at $\tau = 0$.

The reason why $\Pi$ defined in the overdamped regime attains a maximal value in the limit $\tau \to 0$ is as follows. The RTP and ABP active motion is determined by two parameters, the constant magnitude of a swimming velocity $v_0$, and the persistence time $\tau$. In the limit $\tau \to 0$, the swimming direction of an active particle changes very fast. As a result, an active motion fails to produce a net displacement in a particle position. This, effectively, suppresses active motion and explains the emergence of a Boltzmann distribution. The suppression, however, is only apparent and not real, since the magnitude of a velocity in the overdamped regime remains constant. At length scales comparable to or smaller than $v_0\tau$, an active motion can still be detected as a kind of erratic vibration, since the magnitude of a velocity of active motion is constant. And if the volume element where this “vibration” occurs is sufficiently small for an external potential to remain constant, it is as if an active particle found itself in unconfined environment. Unimpeded by any confinement, the entropy production attains a maximal value.

With inertia taken into account, in the regime $\tau \ll \tau_\text{r}$ a swimming velocity fails to adjust itself to a rapidly changing force direction. As a result, the magnitude of a swimming velocity is reduced, and in the limit $\tau \to 0$ it altogether vanishes. And once a velocity (due to active motion) is suppressed, the entropy production rate goes to zero, identifying the limit $\tau \to 0$ as equilibrium.

In addition to the above motivation, the current study is relevant to a growing interest in active particle models with inertia [13–15]. Such models are more representative of particles embedded in low-density environment such as gas. Examples include mesoscopic dust particles in plasmas [16], granulars on a vibrating plate [17], or insect flight at water interfaces [18].

To formulate $\Pi$ within underdamped dynamics, we explore the link between the entropy production rate and the heat dissipation rate [19–23]. From the Kramers equation for particles in an external potential, we obtain a number of alternative formulations of $\Pi$. One by-product of this analysis is the derivation of the virial theorem for active particles. Another interesting result is the representation of stationary distributions in $v$-space, for active particles in unconfined environment and in a harmonic trap, as a convolution between the Maxwell distribution and the distribution at zero temperature. This is possible because in both cases the two random processes are independent. The independence of the random processes is lost for other types of confinements.

Furthermore, this work shows that for particles in a harmonic trap the entropy production is found to be maximal at $\tau = \omega^{-1}$, where $\omega$ is the natural frequency of a harmonic potential. For $\tau < \omega^{-1}$ the entropy production quickly decreases and then vanishes at $\tau = 0$. This suggests the presence of two equilibria, in the limits $\tau \to 0$ and $\tau \to \infty$. The equilibrium in the limit $\tau \to \infty$ represents a system in equilibrium with quenched disorder [24–25]. This is different from analysis based on overdamped dynamics where the entropy production increases monotonically with decreasing $\tau$ and is maximal at $\tau = 0$. Therefore, only a single equilibrium at $\tau \to \infty$ is predicted.

The role of inertia in determining entropy production has been investigated in the past. In [26–27] this was done for a system in the presence of temperature gradients and in [28], for a Brownian particle in a harmonic trap and in contact with two heat baths. To our knowledge, the role of inertia on $\Pi$ for active particle systems has been considered for the first time in [6] for an unconfined environment and in two-dimensions, and without considering the RTP model. More recently, some aspects of inertia within the AOUP model were considered in
II. ENTRPY PRODUCTION AS A DISSIPATION OF HEAT

The second law of thermodynamics states that a non-reversible process is characterized by the production of entropy. The process of entropy production is commonly represented as \[ S = Π - Φ, \]

where \( S \) is the time derivative of the entropy, \( Π \) is the entropy production rate, and \( Φ \) is the entropy flux in and out of the system that occurs in two forms: heat transfer \( q/T \) and mass flow. Without mass flow, the entropy flux simply is

\[ Φ = \frac{q}{T}, \]

and for the stationary state \( \dot{S} = 0 \), Eq. (1) leads to

\[ TΠ = \dot{q}, \]

establishing a relation between entropy and heat production \cite{20, 21, 33, 35}.

III. LANGEVIN EQUATION ANALYSIS

In this work we consider particles whose velocity evolves according to the following (underdamped) Langevin equation

\[ \tau_c \dot{v} = -v + η + µf + µF, \]

where \( \tau_c = mμ/κ_B \) is the inertial relaxation time, \( m \) is the mass of a particle, and \( μ \) is the mobility. The two stochastic processes are thermal fluctuations \( η \) and the force \( f \) that is responsible for generating active motion. The two systematic forces are \( F \), an external position dependent force, and the drag force \( F_d(t) = -v(t)\mu^{-1} \) due to a surrounding fluid. Using a definition of power, \( P_r = v \cdot F \), we get the heat dissipation rate \( \dot{q}(t) = v^2(t)\mu^{-1} \), which is proportional to the kinetic energy of a particle.

Thermal fluctuations \( η \) are represented as a Gaussian white noise which on average imparts a fixed amount of energy \( E_k = \frac{κ_B}{2}T \), where \( n \) is the system dimension, \( T \) is a thermal temperature, and \( κ_B \) is the Boltzmann constant.

Dissipation of energy means absorption of heat by an infinite reservoir so that the temperature of a finite system does not rise. The energy that comes from the reservoir in form of thermal fluctuations is not really dissipated since at another time it is returned to a particle as thermal noise. Only the part of a kinetic energy that comes from \( f \) is truly dissipated. This means that when calculating the average dissipation of heat, the contribution that comes from thermal fluctuations needs to be subtracted. This results in the following formula of the dissipation of heat:

\[ TΠ ≡ ⟨q⟩ = \frac{1}{μ} \left[ ⟨v^2⟩ - \frac{nD}{τ_c} \right], \quad \text{RTP and ABP}, \]

where \( D = μκ_BT \) is the diffusion constant and \( τ_c = mμ/κ_B \) is the inertial relaxation time. The above formulation is the centerpiece of this article. In subsequent sections, this formula, and its alternative manifestations, will be used to calculate \( Π \) for different scenarios. The fact that contributions of \( η \) to the kinetic energy remain the same, regardless of the presence of active motion or any external potential, is a consequence of \( η \) being independent of \( f \) and \( F \). This independence will be demonstrated more rigorously in the next section.

It is possible at this stage to propose an alternative formulation of \( ⟨q⟩ \) by multiplying the Langevin equation in Eq. (4) by \( v \) and taking average. This leads to

\[ \frac{τ_c}{2} \left\langle \frac{dv^2}{dt} \right⟩ = -⟨v^2⟩ + ⟨v \cdot η⟩ + μ⟨v \cdot f⟩ + μ⟨v \cdot F⟩. \]

The term on the left-hand-side represents flux of the kinetic energy in and out of the system and for a stationary state it is zero \cite{36, 38}. The second term on the right hand side evaluates to \( ⟨v \cdot η⟩ = nD/τ_c \) (this relation will be derived again later from the stationary Kramers equation). Finally, the last term representing power input due to an external potential vanishes, \( ⟨v \cdot F⟩ = 0 \), since the external force on average does not contribute to the production of energy in a stationary state. (This relation will also be derived later from the Kramers equation.)

Using these results, Eq. (6) together with Eq. (5) leads to another definition of the dissipation of heat based on the average power input:

\[ TΠ ≡ ⟨q⟩ = ⟨v \cdot f⟩. \]

Later we derive two other formulations of \( ⟨q⟩ \) from the Kramers stationary equation.

The interpretation of heat dissipation as a result of an external time dependent force \( f \) poses no problems for the RTP and ABP models, for which this interpretation was originally intended. In the case of the AOUP model, the force \( f \) is represented as a colored noise \cite{41, 42}:

\[ μf = \frac{1}{τ_c} \int_{-∞}^{t} ds e^{-(t-s)/τ_c} η_f(s), \quad \text{AOUP}, \]

where \( η_f \) is a white noise where the subscript "f" is used to distinguish this noise from the white noise of a reservoir. But note that in the limit \( τ_c → 0 \), \( μf → η_f \), which recovers the standard Langevin equation for a passive Brownian motion, \( τ_c → 0 \), however, with two sources of white noise and, as a result, an enhanced thermal temperature \( T → T + T_f \).

This raises a question: should we regard \( η_f \) as an external time dependent noise, or do we regard it as a thermal fluctuation, in which case we must postulate, and justify, the existence of a second reservoir. To treat all models uniformly, in this work we always consider \( f \) as a force with an external source. The ambiguity that arises for the AOUP model does not affect a number of different relations that are later obtained. The main motivation of this work is to understand inertia effects in the RTP and ABP models, for which there is no ambiguity of interpretation, on the entropy production rate.
IV. UNCONFINED ENVIRONMENT

To obtain an expression for $\Pi$ as defined in Eq. (5), we need to calculate the variance $\langle v^2 \rangle$, which can be obtained by solving the Langevin equation:

$$
\langle v^2 \rangle = \frac{1}{\tau_\v} \int_0^\tau ds \int_0^s ds' e^{-(s-s')/\tau_\v} e^{-(s'-s'/\tau_\v} \langle \eta(s) \cdot \eta(s') \rangle \nonumber
$$

$$
\times \left[ \langle \eta(s) \cdot \eta(s') \rangle + \mu^2 \langle f(s) \cdot f(s') \rangle + \mu^2 \langle F(s) \cdot F(s') \rangle + 2\mu \langle f(s) \cdot \eta(s') \rangle + 2\mu \langle F(s) \cdot \eta(s') \rangle + 2\mu^2 \langle F(s) \cdot F(s') \rangle \right].
$$

Because thermal fluctuations are independent of all the forces, $\langle f(t) \cdot \eta(t') \rangle = \langle F(t) \cdot \eta(t') \rangle = 0$, the contributions of thermal fluctuations to $\langle v^2 \rangle$ are always the same and is given by

$$
\langle v^2 \rangle_{\text{eq}} = \frac{1}{\tau_\v} \int_0^\tau ds \int_0^s ds' e^{-(s-s')/\tau_\v} e^{-(s'-s'/\tau_\v} \langle \eta(s) \cdot \eta(s') \rangle,
$$

which evaluates to $\langle v^2 \rangle_{\text{eq}} = nD/\tau_\v$. This is the reason why in Eq. (5) we subtracted the quantity $nD/\tau_\v$ from $\langle v^2 \rangle$.

For an unconfined environment $F = 0$, the expression in Eq. (9) can be evaluated considering that the two random processes are uncorrelated, $\langle f(t) \cdot \eta(t') \rangle = 0$, thermal fluctuations are delta correlated, $\langle \eta(t) \cdot \eta(t') \rangle = 2nD\delta(t-t')$, and the force $f$ is exponentially correlated, $\langle f(t) \cdot f(t') \rangle = \langle f^2 \rangle e^{-(t-t')/\tau}$, where $\tau$ is the persistence time. The evaluated expression is

$$
\langle v^2 \rangle = \frac{\mu^2 \langle f^2 \rangle}{1 + \tau / \tau_\v} + \frac{nD}{\tau_\v}.
$$

(11)

Inserting this into Eq. (5) and using expressions for $\langle f^2 \rangle$ in Eq. (13), the relation yields

$$
T\Pi \equiv \langle \dot{q} \rangle = \mu \langle f^2 \rangle \frac{\tau}{\tau + \tau_\v}
$$

(12)

In the RTP and ABP models the magnitude of $f$ is constant, $|f| = v_0/\mu$, and we have

$$
\langle f^2 \rangle = \frac{v_0^2}{\mu^2}, \quad \text{RTP and ABP},
$$

(13)

where $v_0$ represents a swimming velocity that a particle would attain in the overdamped regime in response to the force $f$. $v_0$ should not to be confused with the actual velocity $v = |v|$. Inserting this in Eq. (12) results in

$$
T\Pi \equiv \langle \dot{q} \rangle = \frac{v_0^2}{\mu} \frac{\tau}{\tau + \tau_\v}, \quad \text{RTP and ABP}.
$$

(14)

The formula for $\langle \dot{q} \rangle$ is independent of thermal fluctuations. For overdamped dynamics, $\tau_\v = 0$, the heat dissipation becomes independent of $\tau$. The inclusion of inertia leads to reduced dissipation as a function of decreasing $\tau$, where in the limit $\tau \to 0$ the dissipation vanishes, indicating that a system is in equilibrium.

In the AOP model, the force $f$ evolves as $\dot{f} = -f + \eta_f \mu^{-1}$, where $\eta_f$ is a delta correlated Gaussian noise, $\langle \eta_f(t) \cdot \eta_f(t') \rangle = 2nD\delta(t-t')$, and $D_f$ is the diffusion constant of that process. This results in

$$
\langle f^2 \rangle = \frac{nD_f}{\tau f_\mu}, \quad \text{AOUP}.
$$

(15)

Inserting this in Eq. (12) leads to

$$
T\Pi \equiv \langle \dot{q} \rangle = \frac{nD_f}{\mu} \frac{1}{\tau + \tau_\v}, \quad \text{AOUP}.
$$

(16)

The absence of the dependence of $\langle \dot{q} \rangle$, in the RTP and ABP models, on the system dimension $n$ can be traced to the quantity $\langle f^2 \rangle$ in Eq. (15), and the fact that the magnitude of the force $f$ is fixed. In contrast, the same quantity for the AOP model depends on a system dimension as a result of Eq. (15). In this case, each component of the vector $f$ evolves independently.

The result in Eq. (14) and in Eq. (16) are in agreement with those in [6] (Table 1 in that reference) using different derivation. The results in [6] are limited to 2D, but the formula in Eq. (14) and Eq. (16) apply to any system dimension.

A. "Maxwell" distributions of active particles in unconfined environment

From Eq. (11), it can inferred that $\langle v^2 \rangle$ is a sum of two contributions:

$$
\langle v^2 \rangle = \langle v^2 \rangle_{\text{eq}} + \langle v^2 \rangle_{\text{ac}},
$$

(17)

where $\langle \ldots \rangle_{\text{eq}}$ is an average over thermal fluctuations (without active motion) and $\langle \ldots \rangle_{\text{ac}}$ is an average due to active motion at zero temperature. Such a decomposition of a second moment is a signature of a distribution generated by convolution, $p(v) = \int dv' p_{\text{ac}}(v') p_{\text{eq}}(v - v')$, where

$$
p_{\text{eq}}(v) = \left( \frac{\tau_v}{2\pi D} \right)^{\frac{3}{2}} e^{-\frac{(v)}{2\tau_v}},
$$

(18)

is the Maxwell-Boltzmann distribution (we recall that $D = \mu k_B T$ and $\tau_v = \mu \eta$).

Eq. (18) together with the convolution relation leads to the following distribution in the velocity-space:

$$
p(v) = \left( \frac{\tau_v}{2\pi D} \right)^{\frac{3}{2}} \int dv' p_{\text{ac}}(v') e^{-\frac{(v'-v)}{2\tau_v}^2},
$$

(19)

where $p_{\text{ac}}$ depends on a particular model. A similar convolution formula has recently been determined for active particles in a harmonic trap [25]. Since the Langevin equation in (4) for an unconstrained environment, $F = 0$, can be interpreted as the Langevin equation for an active particle in a harmonic trap in the overdamped regime, we expect an analogous convolution relation to apply in this case.
Convolution arises when the contributing random processes are independent. This is the case for the process represented by the sum $f + \eta$. A more rigorous proof of the convolution relation based on Fourier analysis is provided in appendix (A).

To determine the distribution $p(v)$, we still need an expression for $p_{ac}(v)$. For the RTP model in dimensions $n = 1, 2$, $p_{ac}$ is represented by a beta distribution

$$
p_{ac}(v) \propto \left(1 - \frac{v^2}{v_0^2}\right)^{\frac{1}{2}} \text{RTP for } n = 1, 2.
$$

The above distribution vanishes for $v > v_0$ and exhibits a crossover at $v/v_0 = n/2$, at which point the distribution changes from convex to concave from. In other words, for long persistence times, $v/v_0 > n/2$, velocities accumulate near $v = v_0$, and for shorter persistence times, $v/v_0 < n/2$, velocities accumulate around $v = 0$.

The beta distribution in Eq. (20) is not valid for the RTP model in dimensions $n > 3$. Likewise, there is no simple closed form formula of $p_{ac}$ for the ABP model in any dimension. For the ABP model in 2D, $p(v)$ can be represented as a series solution involving Laguerre polynomials, see Eq. (11) in [43], but there is no such solution at zero temperature or $p_{ac}$. For those cases where $p_{ac}$ is not available, the convolution formula in Eq. (15) can still be used, but the distributions $p_{ac}$ need to be obtained from a simulation.

For the AOUP model, $p_{ac}$ in any dimension is a Gaussian function

$$
p_{ac}(v) \propto e^{-\frac{v^2}{2\tau_0^2}} \text{ AOUP.}
$$

Then application of the convolution relation leads to

$$
p(v) \propto e^{-\frac{v^2}{2\tau_0^2}} \text{ AOUP.}
$$

Note that for $\tau = 0$ the distribution in Eq. (22) does not recover the Maxwell distribution $p_{eq}$ in Eq. (18), complicating an interpretation of such a system as equilibrium.

V. PARTICLES IN CONFINEMENT

To analyze active particles in confinement in the underdamped regime, we consider the Kramers equations [44] for the evolution of $p(r, v, f)$:

$$
\frac{\partial p}{\partial t} = -\nabla_r \cdot \mathbf{v} p - \frac{\partial}{\partial \mathbf{v}} \cdot \left[ (\mu \mathbf{F} - \mathbf{v} + \mu \mathbf{f}) \right] p + \frac{D}{\tau_0^2} \nabla_v^2 p
+ \frac{1}{\tau} \left\{ \frac{\partial}{\partial \theta} (\int_0^{2\pi} d\theta \mathbf{f}_g) - \langle g \rangle \right\} \text{ RTP}
\frac{\partial p}{\partial t} = -\nabla_r \cdot \mathbf{v} p + \frac{D}{\tau_0^2} \nabla_v^2 p, \text{ ABP}
\nabla_r \cdot \mathbf{f}_p + \frac{D}{\tau_0^2} \nabla_v^2 p, \text{ AOUP.}
\n\mathbf{V}_r, \mathbf{V}_v, \text{ and } \mathbf{V}_f \text{ in Eq. (23) are the gradient operators with respect to } \mathbf{r}, \mathbf{v}, \text{ and } \mathbf{f}, \text{ and } \mathbf{F} = -\mathbf{V} \text{ is the external time independent force. The last terms in Eq. (23) govern the evolution of } \mathbf{f} \text{ and depend on a specific model. For the RTP and ABP models, these terms are defined for a system in two-dimensions to simplify expressions.}

To calculate $\langle v^2 \rangle$, or other average quantities of interest, we multiply the stationary Kramers equation, $\dot{p} = 0$, by a function $g = g(r, v, f)$ and then integrate each term as $\int d\mathbf{r} d\mathbf{v} f d\mathbf{f}$. Using integration by parts, the terms of the Kramers equation are represented as average quantities, $\langle \ldots \rangle = \int d\mathbf{r} d\mathbf{v} f d\mathbf{f} \langle \ldots \rangle$.

$$
0 = \langle \mathbf{v} \cdot \nabla_v g \rangle + \frac{1}{\tau_0} \left\{ \left( \frac{\partial}{\partial \theta} (\int_0^{2\pi} d\theta \mathbf{f}_g) - \langle g \rangle \right) \right\}, \text{ RTP}
+ \frac{1}{\tau} \left\{ \left( \frac{\partial}{\partial \theta} (\int_0^{2\pi} d\theta \mathbf{f}_g) - \langle g \rangle \right) \right\} \text{ ABP}
\langle \mathbf{f} \cdot \nabla_v g \rangle + \frac{D}{\tau_0^2} \langle \nabla_v^2 g \rangle, \text{ AOUP.}
\n\text{Eq. (24) is a template from which various relations can be generated by specifying the function } g. \text{ As we are interested in } \langle v^2 \rangle, \text{ a logical choice seems to be } g = v^2, \text{ which together with Eq. (24) yields}

$$
0 = \langle \mathbf{F} \cdot \mathbf{v} \rangle - \langle v^2 \rangle + \frac{nD}{\tau_0}, \text{ (25)}
$$

The above equation looks similar to Eq. (6) obtained from the Langevin equation. Comparing the two equations, we confirm that $\langle \eta \cdot \mathbf{v} \rangle = \frac{nD}{\tau_0}$.

From the above relation it is obvious that for $\mathbf{f} = 0$ we get $0 = \langle \mathbf{F} \cdot \mathbf{v} \rangle$. To confirm that this result holds for nonzero $\mathbf{f}$ we next use $g = V$. Eq. (24) in this case yields

$$
0 = \langle \mathbf{F} \cdot \mathbf{v} \rangle, \text{ (26)}
$$

which shows the above relation to be valid for any stationary system. We used the relation in Eq. (26) to obtain Eq. (7). Now we provide a more rigorous proof of it.

Combining Eq. (25) with Eq. (26) and using the definition of $\langle q \rangle$ in Eq. (5), we get an alternative formulation of the heat dissipation rate,

$$
\langle q \rangle = \langle \mathbf{f} \cdot \mathbf{v} \rangle, \text{ (27)}
$$

which already was obtained in Eq. (7).

Other formulations of $\langle q \rangle$ are still possible. Inserting $g = \mathbf{f} \cdot \mathbf{v}$ into Eq. (24) yields

$$
0 = \frac{\mu}{\tau_0} \langle \mathbf{F} \cdot \mathbf{f} \rangle - \frac{1}{\tau_0} \langle \mathbf{F} \cdot \mathbf{v} \rangle + \frac{\mu}{\tau_0} \langle f^2 \rangle - \frac{1}{\tau} \langle \mathbf{f} \cdot \mathbf{v} \rangle. \text{ (28)}
$$

Together with Eq. (27), Eq. (28) leads to another formulation of the heat dissipation rate:

$$
\langle q \rangle = \left[ \mu \langle f^2 \rangle + \mu \langle \mathbf{F} \cdot \mathbf{f} \rangle \right] \frac{\tau}{\tau + \tau_0}. \text{ (29)}
$$

The second term can be interpreted as representing contributions of confinement. The correlations between vectors $\mathbf{F}$ and $\mathbf{f}$ are shown in the next section which treats a harmonic confinement to be negative. This means that confinement reduces dissipation. The negative correlations also explain the accumulation of active particles near a trap border.
Another formulation of heat dissipation is obtained by using \( g = r \cdot f \). Eq. (24) in this case yields
\[
0 = (f \cdot v) - \frac{1}{\tau} (f \cdot r).
\]
In combination with Eq. (27) this leads to
\[
\langle \dot{q} \rangle = \frac{1}{\tau} (f \cdot r),
\]
the fourth formula of heat dissipation.

All formulations for the heat dissipation rate are listed below:
\[
T \Pi \equiv \langle \dot{q} \rangle = \begin{cases} 
\frac{1}{\mu} \left[ \langle v^2 \rangle - \frac{\mathbf{a} \mathbf{D}}{\tau} \right] \\
\frac{\mu \langle f^2 \rangle + \mu (\mathbf{F} \cdot \mathbf{f})}{\tau + \tau_r} \\
\frac{1}{\tau} (f \cdot r).
\end{cases}
\]
Note that the second and fourth formulas do not directly depend on the velocity and so apply to models in the overdamped regime.

The stationary distribution \( \rho \) is a function of three vector variables, \( \rho \equiv \rho(\mathbf{r}, \mathbf{v}, \mathbf{f}) \). As shown above, \( \mathbf{f} \) is not an independent variable. It is on average correlated with other vector variables \( (\mathbf{f} \cdot \mathbf{r}) \) and \( \langle \mathbf{f} \cdot \mathbf{v} \rangle \), where the magnitude of correlations is related to the dissipation of heat. To determine correlations between \( \mathbf{r} \) and \( \mathbf{v} \), we insert \( g = r^2 \) into Eq. (24). The result is
\[
0 = (r \cdot v)
\]
indicating the absence of correlations for this pair of vectors.

VI. THE VIRIAL THEOREM OF ACTIVE PARTICLES

In this section, we are going to use Eq. (24) to obtain a virial theorem for active particles. Using \( g = r \cdot f \), Eq. (24) yields
\[
0 = \langle v^2 \rangle + \frac{\mu}{\tau_r} \langle \mathbf{F} \cdot \mathbf{r} \rangle = \frac{\tau}{\tau_r} \langle \mathbf{r} \cdot \mathbf{v} \rangle + \frac{\mu}{\tau_r} \langle \mathbf{f} \cdot \mathbf{r} \rangle.
\]
Together with Eq. (31), Eq. (5), and Eq. (33) the above equation can be expressed as
\[
-\langle \mathbf{F} \cdot \mathbf{r} \rangle = 2\langle E_k \rangle + \tau \langle \dot{q} \rangle,
\]
where \( \langle E_k \rangle = \langle m v^2 / 2 \rangle \) is the average kinetic energy where we used \( \tau_r = m \mu \) to eliminate \( \tau_r \). The relation in Eq. (35) is the virial theorem for active particles. Since at equilibrium the virial theorem is \( -\langle \mathbf{F} \cdot \mathbf{r} \rangle = 2\langle E_k \rangle \), the term \( \tau \langle \dot{q} \rangle \) in Eq. (35) can be regarded as a measure of violation of the virial relation.

The virial theorem in Eq. (35) can be expressed differently by using the fourth formulation in Eq. (32), leading to
\[
-\langle (\mathbf{F} + f) \cdot \mathbf{r} \rangle = 2\langle E_k \rangle.
\]
Given that \( f \) is an external force, the formulation above appears to conform with the original virial theorem.

A virial relation is often considered for the following external potential \( V = Kr^2/s \). In this case \( \mathbf{F} \cdot \mathbf{r} = -s \mathbf{V} \) and Eq. (35) becomes
\[
s\langle \mathbf{V} \rangle = 2\langle E_k \rangle + \tau \langle \dot{q} \rangle.
\]
Active particles for this class of potentials have been studied in [40]. The virial theorem has been previously derived specifically for the AOUP model and using other derivation techniques, see Eq. (28) in [29]. The formulation in this work extends this result to all active particle models.

VII. PARTICLES IN A HARMONIC TRAP

In this section we focus on a specific confining potential, a harmonic trap, resulting in the linear external force \( \mathbf{F} = -K \mathbf{r} \). To obtain an expression for the dissipation of heat, we use Eq. (29). And to obtain an expression for \( \langle \mathbf{F} \cdot \mathbf{f} \rangle \), we substitute into Eq. (24) \( g = \mathbf{F} \cdot \mathbf{f} \). This yields
\[
0 = \langle \mathbf{v} \cdot \nabla_r (\mathbf{f} \cdot \mathbf{f}) \rangle - \frac{1}{\tau} (\mathbf{F} \cdot \mathbf{f}).
\]
For \( \mathbf{F} = -K \mathbf{r} \) the first term becomes \( \langle \mathbf{v} \cdot \nabla_r (\mathbf{f} \cdot \mathbf{f}) \rangle = -K \langle \mathbf{v} \cdot \mathbf{f} \rangle \), then using Eq. (27), Eq. (38) can be written as
\[
\langle \mathbf{F} \cdot \mathbf{f} \rangle = -\tau K \langle \dot{q} \rangle.
\]
Note that the correlations between the vectors \( \mathbf{F} \) and \( \mathbf{f} \) are demonstrated to be negative.

Substituting this result into Eq. (29), the heat dissipation formula for a harmonic trap becomes
\[
T \Pi \equiv \langle \dot{q} \rangle = \mu \langle f^2 \rangle \frac{\tau}{\tau + \tau_r^2 \mu K + \tau_r}.
\]
Then using Eq. (13), we get the dissipation of heat for the RTP and ABP models:
\[
T \Pi \equiv \langle \dot{q} \rangle = \frac{\tau}{\mu} \frac{\tau}{\tau + \tau_r^2 \mu K + \tau_r}, \quad \text{RTP and ABP.}
\]
The entropy production rate for RTP particles in a harmonic trap have previously been obtained for the overdamped regime, or \( \tau_r = 0 \), in [10] [12]. The formulas in Eq. (41) recover these results by setting \( \tau_r \) to zero.

Similar to the case of a unconfined system, \( \langle \dot{q} \rangle \) is independent of temperature. The role of confinement, regulated by the parameter \( K \), is to reduce a dissipation effect. Because the term that depends on confinement is \( \tau^2 \mu K \), the effects of confinement becomes negligible as \( \tau \) becomes small and the dissipation is similar to that in an unconfined environment.

In Fig. (1) we plot simulation data points for \( \langle \dot{q} \rangle \) as a function of \( \tau \) for the RTP and ABP models, different system dimensions, and different temperatures. According to Eq. (41), all points are expected to collapse onto a single curve, which is confirmed by the results. To calculate \( \langle \dot{q} \rangle \), we can use any of the formulas in Eq. (32). All the formulas were tested and shown to yield the same results.
FIG. 1. The heat dissipation rate of self-propelled particles in a harmonic trap as a function of $\tau$. Simulation data points come from four systems. Sim-1 is for RTP particles in 2D and $D = 0$, sim-2 is for RTP particles in 1D and $D = 0.1$, sim-3 for ABP particles in 2D and $D = 0.2$, and sim-4 for ABP particles in 3D and $D = 0.2$. All points collapse onto the curve given by the formula in Eq. (41). The dashed line is $\langle \dot{q} \rangle$ for the overdamped regime. Maximum dissipation occurs at $\tau_{\text{max}} = \sqrt{m/K}$, for the specific parameters of the plot corresponding to $\tau_{\text{max}} = \sqrt{0.1}$.

The simulation data points are compared against $\langle \dot{q} \rangle$ for overdamped dynamics, obtained from Eq. (41) with $\tau_r = 0$. The two curves deviate in the region $\tau \leq \tau_c$. As $\langle \dot{q} \rangle$ quantifies a distance from equilibrium, this leads to different interpretation of the same system when analyzed using different theoretical frameworks.

As seen in Fig. 1, the maximal dissipation of heat for the underdamped regime occurs at non-zero persistence time, corresponding to $\frac{dt_r}{dt} = 0$ and that can be calculated using Eq. (41), yielding

$$\tau_{\text{max}} = \sqrt{\frac{m}{K}} = \omega^{-1},$$

where $\omega$ is the natural frequency of an oscillator. This result might be expected based on what is known about driven harmonic oscillators.

Using Eq. (40) and Eq. (15), we get the heat dissipation formula for AOUP particles in harmonic trap:

$$T\Pi \equiv \langle \dot{q} \rangle = \frac{nD_f}{\mu} \frac{1}{\tau_c^2 + 2\tau_c^2 \mu K + \tau_r^2}, \quad \text{AOUP. (43)}$$

As in the case of unconfined system, the expressions for $\langle \dot{q} \rangle$ for the RTP and ABP models in Eq. (41) does not depend on a system dimension $n$. This has to do with the fact that the magnitude of the force vector $f$ is fixed. In contrast, Eq. (43) shows dependence on a system dimension since the vector components of $f$ evolve independently, see Eq. (15).

A. "Maxwell" distributions of active particles in a harmonic trap

Because Eq. (40) is independent of temperature, this implies that the variance can be written as $\langle \dot{q}^2 \rangle = \langle \dot{q}^2 \rangle_{\text{eq}} + \langle \dot{q}^2 \rangle_{\text{ac}}$ which, in turn, implies that a distribution in $\dot{q}$ space obeys the convolution formula $p(\dot{q}) = \int d\dot{q}' p_{ac}(\dot{q}')p_{eq}(\dot{q} - \dot{q}')$ as for the case of unconfined environment in Eq. (19).

The validity of the convolution formula implies that the independence of the random processes $f$ and $\eta$ is not violated by the presence of a linear force of a harmonic trap. In any other type of external potential, the independence of the two processes can no longer be assumed. A more technical demonstration of the validity of the convolution relation for particles in a harmonic trap is given in appendix (15) using Fourier transform analysis.

For the RTP and ABP models, there are no exact expressions for $p_{ac}$ for particles in a harmonic trap, and these distributions need to be obtained from a simulation. For the AOUP model, $p_{ac}(\dot{q})$ is a Gaussian function [39]. Given the value of $\langle \dot{q}^2 \rangle_{\text{ac}}$ in Eq. (43), we know that this function must be given by

$$p_{ac}(\dot{q}) \propto e^{-\frac{\dot{q}^2 + \dot{q}^2}{\mu K} \tau_c^2}, \quad \text{AOUP. (44)}$$

Using the convolution formula in Eq. (19) we then get

$$p(\dot{q}) \propto e^{-\frac{\dot{q}^2}{\mu K} \tau_c^2 + \frac{\dot{q}^2}{\tau_c \tau_r + \tau_c^2 \mu K}}, \quad \text{AOUP. (45)}$$

VIII. RTP MODEL IN 1D BOX

A frequently studies system of active particles are RTP particles in 1D box. In the overdamped regime, the model has been frequently studied and is well understood [9, 46–51]. For underdamped dynamics, the system is governed by the Kramers equation resulting in two coupled differential equations:

$$\dot{p}_+ = -v \frac{\partial p_+}{\partial x} + \frac{1}{\tau_r} \frac{\partial}{\partial y} [(v - v_0) p_+] + \frac{D}{\tau_c} \frac{\partial^2 p_+}{\partial y^2} - \frac{1}{2} \tau_r \left( p_+ - p_- \right)$$

$$\dot{p}_- = -v \frac{\partial p_-}{\partial x} + \frac{1}{\tau_r} \frac{\partial}{\partial y} [(v + v_0) p_-] - \frac{D}{\tau_c} \frac{\partial^2 p_-}{\partial y^2} + \frac{1}{2} \tau_r \left( p_+ - p_- \right),$$

where $p_+(x,v,t)$ and $p_-(x,v,t)$ are the distributions for particles subject to a forward and backward force. The entropy production for this model in the overdamped regime, or $\tau_r = 0$, has been obtained in [9]. For the walls located at $x = \pm h$ it reads

$$T\Pi = \langle \dot{q} \rangle = \frac{v_0}{\mu} \left[ \frac{D}{v_0^2 \tau} \frac{\cosh(kh) - \sinh(kh)}{k^2} \right], \quad \text{(47)}$$

where $k = \frac{v_0}{D} \sqrt{1 + \frac{D^2}{v_0^2 \tau}}$. We can re-derive this result using one of the formulas in Eq. (32), which further demonstrates the accuracy of those formulas.

To calculate $\langle \dot{q} \rangle$ for the underdamped regime, we use the last formula in Eq. (32), which for the present model becomes

$$T\Pi = \frac{v_0}{\tau \mu} [\langle x \rangle_+ - \langle x \rangle_-], \quad \text{(48)}$$
where \((\ldots)_{\pm} = \int_{-\infty}^{\infty} dx \langle \ldots \rangle_{\pm} p_{\pm} \).

Since distributions \(p_{\pm}\) in Eq. (46) cannot be solved exactly, we use simulation to evaluate the expression in Eq. (47). Interaction with the walls is accounted for as follows: each time a particles reaches a wall, its instantaneous velocity changes as \(v(t) \rightarrow -v(t)\). The data points for \(\langle q \rangle\) obtained from a simulation are plotted in Fig. (2). For \(\tau > 2\), the simulation results agree with the exact formula in Eq. (48) for the overdamped regime.

For particles in unconfined environment and in a harmonic trap, the dissipation of heat was found to be independent of temperature. In contrast, for particles in 1D box we observe strong temperature dependence, and the indication that thermal fluctuations reduce dissipation of heat (the difference between the black and red curves).

Interactions of a particle with a wall are analogous to a bouncing ball in the air (within the time duration in which the force \(f\) does not change its direction). Due to air friction, a maximum height at each bounce is lower and the overall velocity reduced. Since interactions with the walls reduce velocity of a particle (and, therefore, the dissipation of heat), increased thermal fluctuations can be seen as contributing to greater number of collisions with the walls. In fact, any type of confinement, other than a harmonic trap, will show a similar reduction of heat dissipation with increased temperature. This was verified by simulations carried out for different trapping potentials of the form \(U \propto r^2\).

There is another interesting feature that arises as a consequence of underdamped dynamics. Within the overdamped regime and at zero temperature, a fraction of particles becomes adsorbed onto confining walls due to the combination of overdamped dynamics and finite persistence time [51]. These particles that are not adsorbed are uniformly distributed within the box [52]. Within the underdamped dynamics, particles coming against a wall no longer become immediately adsorbed. Instead, they are reflected from it, and if the persistence time is sufficiently long, they change direction and come toward the wall again, creating a behavior analogous to bouncing of a ball. As a result, stationary distributions inside the box develop interesting structure shown in Fig. (3). This structure has nothing to do with the size of particles and is entirely a dynamical phenomenon.

Fig. 2. The heat dissipation rate as a function of \(\tau\) for the RTP particles in 1D confined between two walls located at \(x = \pm h\). Dashed lines represent the exact expression in Eq. (47) for the overdamped regime, and the data points for a finite \(\tau\) are obtained from the simulation.

**FIG. 3.** A stationary distribution of RTP particles inside a 1D box at zero temperature. The other system parameters are \(h = \tau = \tau_r = 1\). The distribution is obtained from a simulation.

**IX. CONCLUSION**

In this work we calculate the entropy production rate in the underdamped regime for all canonical models of active particles in all dimensions and for different confinements. To calculate \(\Pi\), we explore the link between the entropy production rate and the dissipation of heat, which results in Eq. (5) and from which alternative formulations are obtained in Eq. (52) by analyzing the Kramers equation.

Exact results are obtained for particles in a harmonic trap and in unconfined environment. In those two cases, the two random processes \(\eta\) and \(f\) remain independent which permits us to represent the "Maxwell" distribution \(p(v)\) to be represented as a convolution relation. For a harmonic potential, the maximum dissipation of heat occurs for \(\tau = \sqrt{m/K}\). The dissipation of heat vanishes for \(\tau = 0\) and in the limit \(\tau \to \infty\).

For other forms of confinement the two random processes \(\eta\) and \(f\) are generally not independent and as a result the dissipation of heat is found to be reduced as a result of thermal fluctuations.

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**X. DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding author upon reasonable request.
Appendix A: Convolution formulation for an unconfined environment

The convolution formulation of the distribution \( p(v) \) can be demonstrated by analyzing the stationary Fokker-Planck equation for the evolution of \( \rho(v,f) \):

\[
0 = \frac{1}{\tau} \nabla_v \cdot [(v - \mu f) \rho] + \frac{D}{\tau^2} \nabla^2_v \rho + \frac{1}{\tau} \left( \frac{1}{\tau} \frac{\partial}{\partial \theta} \frac{2\pi}{\theta} f \theta \right) \rho \quad \text{RTP}
\]

\[
+ \frac{1}{\tau} \left( \frac{1}{\tau} \frac{\partial}{\partial \theta} \frac{2\pi}{\theta} f \theta \right) \rho \quad \text{ABP}
\]

\[
\frac{\nabla_v \cdot \rho f + D_f \nabla^2_v \rho}{\nabla_v \cdot \rho f + D_f \nabla^2_v \rho} \quad \text{AOUP,}
\]

where the last term determines the evolution of \( f \) and depends on the model. For convenience, these terms are written specifically for 2D where \( f = \mu^{-1} v \mathbf{n} \) (the unit orientation vector \( \mathbf{n} = (\cos \theta, \sin \theta) \) depends only on the angle \( \theta \)). For the AOUP model, \( \nabla_v \cdot f \) is the gradient operator with respect to \( f \).

Taking the Fourier transform of Eq. (A1) with respect to velocity yields

\[
0 = \frac{1}{\tau} [k \cdot \nabla k] - \mu \left[ \frac{1}{\tau^2} + \frac{2\pi i}{\theta} \right] c - \frac{D_k^2}{\tau^2} c
\]

\[
+ \frac{1}{\tau} \left( \frac{1}{\tau} \frac{\partial}{\partial \theta} \frac{2\pi}{\theta} f \theta \right) c - \frac{1}{\tau} \nabla^2_v \pi c \quad \text{AOUP,}
\]

where \( c(k,f) = \int dv \rho(v,f) e^{-ikv} \) and \( c_{eq} \propto e^{-Dk^2/2\tau} \) is the transformed Maxwell distribution. The same equation at zero temperature reads

\[
0 = \frac{1}{\tau} [k \cdot \nabla k] - \mu \left[ \frac{1}{\tau^2} + \frac{2\pi i}{\theta} \right] c_{eq}
\]

\[
+ \frac{1}{\tau} \left( \frac{1}{\tau} \frac{\partial}{\partial \theta} \frac{2\pi}{\theta} f \theta c_{eq} \right) - \frac{1}{\tau} \nabla^2_v \pi c_{eq} \quad \text{AOUP.}
\]

In the Fourier space, the convolution formula in Eq. (19) can be written as

\[
c(k,f) = c_{eq}(k,f) e^{-Dk^2/2\tau}.
\]

Substituting Eq. (A4) into Eq. (A2) splits the first term of that equation into two parts,

\[
\frac{1}{\tau} k \cdot \nabla k e^{-Dk^2/2\tau} = \left( \frac{1}{\tau} k \cdot \nabla k c_{eq} - \frac{D_k^2}{\tau^2} c_{eq} \right) e^{-Dk^2/2\tau}.
\]

where the first term cancels the third term in that equation, recovering Eq. (A3).

The solution in Eq. (A4) not only proves the convolution formula in Eq. (19), but it implies a stronger claim,

\[
\rho(v,f) = \left( \frac{\tau}{2\pi D} \right)^\frac{D}{2} \int d\tau' \rho_{ac}(v,f)e^{-\frac{D}{\tau^2}(v-v')^2},
\]

where \( \rho_{ac} \) is the distribution for \( D = 0 \). Consequently, the effect of temperature on all the distributions \( \rho_{ac} \) is the same. Since \( p(v) = \int df \rho(v,f) \), the above relation proves the convolution in Eq. (19). The proof is valid to all active particle models in unconfined environment.

Appendix B: Convolution formulation for a harmonic trap

In this section we demonstrate that the distribution \( p(v) \) for active particles in a harmonic trap can be represented as a convolution relation between \( p_{ac}(v) \) and \( p_{eq}(v) \). The stationary Kramers equation for particles in a harmonic trap is

\[
0 = -v \cdot \nabla_v \rho + \frac{1}{\tau} \nabla_v \cdot [(\mu K r + v \cdot \mu f) \rho] + \frac{D}{\tau^2} \nabla^2_v \rho + \ldots,
\]

where the terms for the evolution of \( f \), that do not play role in the proof, are ignored. We next take the Fourier transform with respect to \( r \) and \( v \) that yields

\[
0 = q \cdot \nabla_q c - \frac{\mu K}{\tau} q \cdot \nabla q e^{-q r} - \frac{1}{\tau} k \cdot \nabla k c - \frac{\mu}{\tau} [k \cdot f] c - \frac{D_k^2}{\tau^2} c + \ldots
\]

where \( c(q,k,f) = \int d\tau d\sigma \rho(v,f) e^{-iq r} e^{-ikv} \). We next assume the following solution

\[
c = c_{ac} e^{-Dq^2/2\tau} e^{-Dq^2/2\mu K},
\]

where \( e^{-Dq^2/2\tau} \) is a Fourier transformed Maxwell distribution in \( v \)-space and \( e^{-Dq^2/2\mu K} \) is a Fourier transformed equilibrium distribution in positional space. It turns out that if we substitute this function into Eq. (B2), we will eliminate all the terms that depend on \( D \) and recover

\[
0 = q \cdot \nabla_q c_{ac} = \frac{\mu K}{\tau} q \cdot \nabla q c_{eq} - \frac{1}{\tau} k \cdot \nabla k c_{ac} - \frac{\mu}{\tau} [k \cdot f] c_{ac} + \ldots,
\]

which is the same as Eq. (B2) but for \( D = 0 \). This means that Eq. (B3) is a correct solution. In physical space, this implies the following convolution:

\[
\rho(r,v,f) = \int d\tau' \int d\tau'' \rho_{ac}(r',v',f') e^{-\frac{\mu K}{\tau'}(r-r')^2} e^{-\frac{D}{\tau''}(v-v')^2}.
\]

After integrating over \( r \) and \( f \) we recover the convolution in Eq. (19).

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