Effective entropy production and thermodynamic uncertainty relation of active Brownian particles

Cite as: Phys. Fluids **34**, 053310 (2022); https://doi.org/10.1063/5.0094211 Submitted: 01 April 2022 • Accepted: 29 April 2022 • Accepted Manuscript Online: 30 April 2022 • Published Online: 10 May 2022

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ABSTRACT

Understanding stochastic thermodynamics of the active Brownian particles system has been an important topic in very recent years. However, thermodynamic uncertainty relation (TUR), a general inequality describing how the precision of an arbitrary observable current is constraint by energy dissipation, has not been fully studied for a many-body level. Here, we address such an issue in a general model of an active Brownian particles system by introducing an effective Fokker–Planck equation, which allows us to identify a generalized entropy production only by tracking the stochastic trajectory of particles' position, wherein an activity and configuration dependent diffusion coefficient come into play an important role. Within this framework, we are able to analyze the entropic bound as well as TUR associated with any generalized currents in the systems. Furthermore, the effective entropy production has been found to be a reliable measure to quantify the dynamical irreversibility, capturing the interface and defects of motility induced phase separation. We expect the new conceptual quantities proposed here to be broadly used in the context of active matter.

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I. INTRODUCTION

Over the past two decades, stochastic thermodynamics has gained extensive attention for describing nonequilibrium thermodynamics of mesoscopic systems.^{1–5} Due to the small size of such systems, fluctuations are significant, so that thermodynamic quantities become stochastic variables. This observation allows ones to generalize laws of thermodynamics at single trajectory level,^{6–8} which leads to the study of stochastic energetics and fluctuation theorems (FT). In particular, an important universal inequality between the fluctuation in currents and thermodynamic cost, the thermodynamic uncertainty relation (TUR), has been discovered.^{9–17,19–22} Specifically, TURs constrain the Fano factor of an arbitrary observable current by the total entropy production, presenting a trade-off relation between precision and dissipation, and provide an alternative method to obtain a lower bound on the entropy production. Moreover, TURs make an irreplaceable contribution to our understanding of non-equilibrium phenomena (e.g., work extraction under measurement and feedback¹ and biological clocks²⁴), which can provide more detailed information about the systems than the second law. TUR was first proposed for biological processes by Barato and Seifert⁹ and then extended to many other situations, such as diffusion process,^{11,13} finite-time generalization,^{11,12,16} periodically driven systems,^{14,21} biological oscillators,^{17,18,22,25} and time-delayed systems.²⁶

Very recently, the frontiers of stochastic thermodynamics have shifted to the active particle systems. Active particles form a class of nonequilibrium systems, which have the ability to perform directional motion through self-propulsion by consuming energy from the environment.²⁷⁻³⁵ Study of active particles encompasses a wide variety of biological and soft matter systems, such as schools of fish,²⁷ biological microorganisms,^{36–40} and colloidal particles.^{41–43} Such systems can usually show a range of typical collective behaviors, including phase separation,^{44–46} turbulence,^{47–49} and self-assembly.⁵⁰ It has been reported that even the purely repulsive active systems can yield a motility induced phase separation (MIPS) where particles spontaneously separate into solid-like and gas phases,^{30,34} which has attracted much attention. So far, the laws of thermodynamics, the definition of related entropy production, or the construction of fluctuation theorem in active particle systems has been discussed in a few studies.⁵¹⁻⁶⁷ Most studies require not only tracking the particles' position but also full information including the self-propulsion, 54,65-67 which is a great challenge in experiments.⁶⁸ Therefore, how to understand the behaviors of many-body active particle systems from a thermodynamics

perspective in most practical scenarios when only partial information is available, such as the establishment of TUR, is a great challenge.

In this article, based on the approximation of mapping the active particles system to an "effective equilibrium" one,^{69–72} we have introduced a generalized entropy production (EP) S_g , which only needs to track the position of particles. We compare the proposed EP with definitions in other studies and demonstrate the hierarchical order between them by analyzing the degree of coarse-graining. Direct simulations help us to identify the generalized EP at each point in the phase diagram. Detailed analysis of the spatial distributions of the proposed quantity allows us to identify the interface and defects of MIPS, which means that it can unambiguously be utilized to measure the dynamic irreversibility on a macroscopic scale. Furthermore, the entropic bounds^{73,74} and generalized TURs^{9–22,26,67} of active systems based on the demonstrated approximation provide a convenient tool for entropy production inference.⁷⁵

II. MODEL

We consider a homogeneous system of *N* active Brownian particles with spatial coordinates $\mathbf{x}(t) = {\mathbf{x}_i(t)}$, self-propelling with constant velocities $_0$ along its direction of orientations $\mathbf{n}_i = (\cos \theta_i, \sin \theta_i)$ for *i*th particle. Assume that the particles move in a viscous medium and hydrodynamic interactions are neglected, the resulting governing equations are

$$\dot{\boldsymbol{x}}(t) = \mu \boldsymbol{F}(\boldsymbol{x}) + v_0 \boldsymbol{n}(t) + \boldsymbol{\xi}(t), \qquad (1)$$

$$\dot{\theta}_i(t) = \zeta_i(t). \tag{2}$$

Here, $\mathbf{F} = -\nabla_{\mathbf{x}} U$ is the mechanical force generated from the total interactions $U(\mathbf{x})$ and μ is the mobility. The stochastic terms $\xi_i(t)$ and $\zeta_i(t)$ are Gaussian white noises with correlations $\langle \xi_i(t)\xi_j(s) \rangle = 2D_t \delta_{ij}\delta(t-s)$ and $\langle \zeta_i(t)\zeta_j(s) \rangle = 2D_r \delta_{ij}\delta(t-s)$. The translational diffusion coefficient D_t satisfies $D_t = \mu k_B T$, where k_B is the Boltzmann constant (which is set to be 1 throughout the paper) and T is the ambient temperature. The rotational diffusion coefficient D_r relates to persistent time as $\tau_p = (2D_r)^{-1}$. To derive an explicit TUR for the ABPs system, we now introduce a coarse-grained active Ornstein–Uhlenbeck process with thermal noise (AOU-T) as a direct mapping model, which reads

$$\dot{\boldsymbol{x}}(t) = \mu \boldsymbol{F}(\boldsymbol{x}) + \boldsymbol{\xi}(t) + \boldsymbol{\eta}^{A}(t).$$
(3)

Here, the active term $\eta^A(t)$ represents the OU active components with zero mean and time correlation

$$\langle \eta_i^A(t)\eta_j^A(s)\rangle = \frac{v_0^2}{3}e^{-|t-s|/\tau_p}\delta_{ij}.$$
(4)

In the limit $\tau_p \to 0$, the time correlation becomes $\langle \eta_i(t)\eta_j(s) \rangle = 2D_a \delta_{ij} \delta(t-s)$ with $D_a = v_0^2 \tau_p/3$, i.e., the system reduces to an equilibrium one with effective diffusion coefficient $D_t + D_a$.

Over the past decade, study of ABPs is a very hot topic and has gained extensive research attention. In particular, stochastic thermodynamics of ABPs has become a frontier area very recently. The main motivation of the present work is to address a TUR for the many-body ABPs system. Following the scheme proposed by Seifert,² one can define the EP of the system along a given stochastic trajectory $\chi(t) = {\mathbf{x}(t)|_{t=0}^{t=t_f}}$ as $S_{sys}(t) = -\ln P(\mathbf{x}, t)$, where $P(\mathbf{x}, t)$ is the configurational probability distribution for the state variable to take the

value *x* at time *t*. In order to establish the framework of stochastic thermodynamics of many-body active systems, we need to obtain the Fokker–Planck equation (FPE), which governs the evolution of probability distribution P(x, t).⁶⁹ To proceed, we adopt the Fox method^{71,72} to get an effective FPE, which can best approximate the process of physical interest and make accurate predictions,^{77–79} which reads

$$\partial_t P(\mathbf{x}, t) \approx -\sum_{i=1}^N \partial_{x_i} J_i(\mathbf{x}, t).$$
 (5)

The probability current is given by

$$J_i(\mathbf{x},t) = D_i(\mathbf{x})\beta F_i^{eff}(\mathbf{x})P(\mathbf{x},t) - D_i(\mathbf{x})\partial_{x_i}P(\mathbf{x},t),$$
(6)

where $\beta = 1/T$, and $D_i(\mathbf{x})$ denotes a configuration-dependent diffusion coefficient given by

$$D_i(\boldsymbol{x}) = D_t + D_a [1 - \beta \tau \partial_{x_i} F_i(\boldsymbol{x})]^{-1},$$
(7)

where $\tau = \tau_p D_t / d^2$ is a dimensionless persistence time and d is the typical diameter of a particle. $F_i^{eff}(\mathbf{x}) = D_i^{-1}(\mathbf{x})[D_tF_i(\mathbf{x}) - T\partial_{x_i}D_i(\mathbf{x})]$ gives the effective force exerting on the *i*th particle. For a passive system in the absence of $\boldsymbol{\eta}^{A}(t)$, $D_{i}(\boldsymbol{x}) = D_{t}$, and $F_{i}^{eff}(\boldsymbol{x}) = F_{i}(\boldsymbol{x})$, while in the limit $\tau \to 0$, $D_i(\mathbf{x}) = D_t + D_a$ and $F_i^{eff}(\mathbf{x}) = D_t F_i(\mathbf{x}) / (D_t + D_a)$. The Fox method is an approximation, which is valid in lower powers of the persistence time τ_p , as shown in the original paper.^{71,72} Nevertheless, it may go beyond this by including contributions to higher orders in τ_p .^{69,70} Indeed, detailed studies of different systems demonstrate the validity of Fox approximation over a large range of τ_p values.⁷⁶ Thus, one may expect that Fox approximation could be applied in a certain range of τ_p , the exact values of which may be system-dependent. In the current system of active particles, there still exists another condition for the Fox approximation to be valid, i.e., $1 - \beta \tau \partial_i F_i(\mathbf{x}) > 0$, such that $D_i(\mathbf{x})$ is positive in the entire area. Thus, the range of accessible τ_p values depends upon the specific form of the bare interaction potential.

III. EFFECTIVE ENTROPY PRODUCTION

Based on the Fox approximation, the AOU-T equation Eq. (3) corresponds to an equivalent Langevin equation. Within this framework, $F^{eff}(\mathbf{x})$ represents the effective interparticle force done on the particle, which is related to the heat flux of the system. According to Sekimoto's suggestion,¹ we can define a generalized heat dissipation in the medium along a stochastic path $\chi(t)$ as

$$\Sigma_m[\chi] = \int_0^{t_f} \boldsymbol{F}^{eff}(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}} dt, \qquad (8)$$

where " \circ " stands for the Stratonovich product and the superscript "T" means transposition. Since the effective force $F^{eff}(\mathbf{x})$ is the total force done on the system, including the effect of activity, the generalized heat dissipation will recover to the normal heat dissipation $\int_0^{t_f} \mathbf{F}(\mathbf{x})^{\mathrm{T}} \circ \dot{\mathbf{x}} dt$ in passive systems.² The difference between these two types of heat dissipation is the activity-induced extra entropy flux.

According to Eq. (6), the change rate of the system entropy is

$$S_{sys}(t) = -\partial_t \ln P(\mathbf{x}, t),$$

$$= -\frac{1}{P(\mathbf{x}, t)} \left[\frac{\partial P(\mathbf{x}, t)}{\partial t} + \sum_{i=1}^N \partial_{x_i} P(\mathbf{x}, t) |_{\mathbf{x}(t)} \dot{\mathbf{x}}_i \right],$$

$$= -\frac{1}{P(\mathbf{x}, t)} \left[\frac{\partial P(\mathbf{x}, t)}{\partial t} - \sum_{i=1}^N \frac{J_i(\mathbf{x}, t)}{D_i(\mathbf{x})} \Big|_{\mathbf{x}(t)} \dot{\mathbf{x}}_i \right],$$

$$-\beta F^{eff}(\mathbf{x})^{\mathrm{T}} \dot{\mathbf{x}}.$$
 (9)

Clearly, the final term in the third equality is related to the generalized heat dissipation in Eq. (8), i.e., $\beta F^{eff}(\mathbf{x})^{\mathrm{T}} \circ \dot{\mathbf{x}} = \dot{\Sigma}_m/T$. Then, Eq. (9) can be rewritten as a balance equation for the trajectory-dependent total EP $\dot{S}_g = \dot{\Sigma}_m/T + \dot{S}_{sys}$,

$$\dot{S}_g(t) = -\frac{\partial_t P(\mathbf{x}, t)}{P(\mathbf{x}, t)} \bigg|_{\mathbf{x}(t)} - \sum_{i=1}^N \frac{J_i(\mathbf{x}, t)}{D_i(\mathbf{x}) P(\mathbf{x}, t)} \bigg|_{\mathbf{x}(t)} \dot{x}_i.$$
(10)

By averaging over the path ensemble, we can obtain the following equation:

$$\langle \dot{S}_{g}(t) \rangle \approx \sum_{i=1}^{N} \int \frac{J_{i}^{2}(\boldsymbol{x}, t)}{D_{i}(\boldsymbol{x})P(\boldsymbol{x}, t)} d\boldsymbol{x} \ge 0,$$
(11)

where $\int d\mathbf{x} \partial_t P(\mathbf{x}, t) = 0$ and $\langle \dot{x}_i | \mathbf{x}, t \rangle \approx J_i(\mathbf{x}, t) / P(\mathbf{x}, t)$ have been used. All the information about particle activity is contained in $D_i(\mathbf{x})$ and $J_i(\mathbf{x})$. The second law Eq. (11) ensures that the averaged total EP must increase with time. The equality holds if all the currents $J_i(\mathbf{x})$ vanish, i.e., the system can be exactly mapped to an equivalent equilibrium system.

In general, the generalized EP Sg along a stochastic trajectory is an apparent measure of the time-reversal symmetry broken of the system at the scale of observed trajectories. In the current work, the proposed EP can be obtained simply by tracking the trajectory $\chi(t)$ $= \{ \mathbf{x}(t) |_{t=0}^{t=t_f} \}$ for particle positions $\mathbf{x}(t)$. To this end, two steps have been used. First, the orientational degree of freedom n(t) has been eliminated and replaced by a colored noise within a mean-field level of description. Second, the system with a non-Markovian colored noise is approximated to an effective equilibrium one on a coarse-grained timescale via the Fox method. Therefore, the instantaneous entropy production rate (EPR) $\dot{S}_g = F^{eff}(\mathbf{x})^{\mathrm{T}} \circ \dot{\mathbf{x}}/T + \frac{d}{dt} \ln P(\mathbf{x}, t)$ defined in our work can be viewed as a "coarse-grained" measure of dynamic irreversibility of the system (In steady states, $\dot{S}_g = F^{eff}(\mathbf{x})^{\mathrm{T}} \circ \dot{\mathbf{x}}/T$). Based on this effective mapping, a clearcut TUR for the coarse-grained EPR can then be well established. Other frameworks for studying EPR and related properties for the ABPs system have been proposed. Nevertheless, many-body TUR has not been addressed so far. In the following, we elucidate the precise hierarchy of EPs.

First, in Ref. 65, Szamel has proposed an EPR $\dot{S}_{sz} = \dot{\Sigma}_{sz}/T$ + $\frac{d}{dt} \ln P(\mathbf{x}, \mathbf{n}; t)$ for the active particles with the heat dissipation $\dot{\Sigma}_{sz} = (\mathbf{F} + \mu^{-1}v_0\mathbf{n})^{\mathrm{T}} \circ \dot{\mathbf{x}}$. \dot{S}_{sz} was constructed at the full dynamics level described by Eqs. (1) and (2), including the information of orientation trajectory with difficulty in tracking. As discussed above, the generalized heat dissipation rate \dot{S}_g proposed by us can be regarded as a coarse-grained form of \dot{S}_{sz} , since the orientational degree of freedom $\mathbf{n}(t)$ has been reduced and the memory effects have been coarse-grained. The difference between \dot{S}_g and \dot{S}_{sz} is commonly referred to as "hidden EPR," which can be identified as the loss of information quantifying the correlation between particle trajectory and the active term.^{53,63,64,66,80–84}

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Second, based on the AOU-T model Eq. (3), Debalow *et al.* has proposed an instantaneous EPR $\dot{S}_{da} = F_m[\chi, t]^T \circ \dot{\mathbf{x}}/T$ (here $F_m[\chi, t]$ is defined as the nonlocal "memory forces"), which depends not only on $\mathbf{x}(t)$ but also on the whole trajectory $\chi(t) = \{\mathbf{x}(t)|_{t=0}^{t=t_f}\}$ of the particles' position.⁵³ In contrast, according to the definition of generalized EPR in our work, $\dot{S}_g = F^{eff}(\mathbf{x})^T \circ \dot{\mathbf{x}}/T + \frac{d}{dt} \ln P(\mathbf{x}, t)$, one can clearly find that it is only dependent on the current configuration $\mathbf{x}(t)$ in the steady state, which is easily accessible in experiments. On the other hand, since AOU-T model is a coarse-grained form of Eqs. (1) and (2), we also have another EP hierarchy: $\dot{S}_{sz} > \dot{S}_{da}$.

Third, in the literature, various continuous field theories based on coarse-graining procedures have been proposed to capture the large scale physics of active particles, such as "Active Models" A, B, and H.⁸⁸ In Ref. 62, based on Active model B, Nardini *et al.* proposed an EPR S_{na} to quantify the dynamic irreversibility of the many-body active particle systems at a macroscopic scale, even when phase separation happens. Therein, the local steady-state EPR was defined as $S_{na} = -\frac{1}{D} \langle \mu_A \dot{\phi} \rangle$, where $\phi(\mathbf{x}, t)$ denotes the fluctuating density field, μ_A is the additional contribution to the chemical potential due to the effect of activity and *D* is collective diffusivity. Due to its field dependence, S_{na} is more coarse-grained than our version S_g .

At last, to highlight the effect of activity and effective interactions, it would be instructive to consider a comparative case, where one can treat the active system as another "effective equilibrium" system with a high effective temperature $T_{eff} = \mu^{-1}(D_t + D_a)$, corresponding to the case in the limit $\tau_p \rightarrow 0$. The corresponding total EPR is given by $\dot{S}_g^{(1)} = F(\mathbf{x})^{T} \circ \dot{\mathbf{x}}/T_{eff}$. Such scheme has been reported to establish the TUR for a single hot Janus swimmer successfully.⁵⁶ The difference between $\langle \Delta S_g \rangle$ and $\langle \Delta S_g^{(1)} \rangle$, treated as some kind of the "hidden EP" discussed above, is dominant especially when the gradient of mechanical force $\partial_{x_i} F_i(\mathbf{x})$ is significant.

Generally, due to the above discussion, the hierarchical structure of the mentioned EPRs can be rationalized as $\dot{S}_{sz} > \dot{S}_{da} > \dot{S}_g > \dot{S}_g^{(1)} > \dot{S}_{na}$ by clarifying their corresponding degree of coarse-graining. Such a hierarchy has a similar counterpart in Maxwell's demon system.^{90,91}

In the following, we also present some discussion about the physical quantities by our formulation and the Harada-Sasa relation (HSR), which provides a useful tool to calculate the heat dissipation of the nonequilibrium systems.⁸⁵ Specifically, Harada and Sasa proposed an exact equality quantifying heat production in terms of the violation of the fluctuation dissipation relation (FDR), which has been developed for active particle systems. For instance, in Ref. 62, Nardini et al. have derived a generalized HSR within a field-theoretical description of an active matter. Chaki and Chakrabarti have utilized the HSR to calculate the heat dissipation of a colloidal particle immersed in an active bath.⁵⁸ More recently, Jones et al. have analyzed the power dissipation of an active microswimmer (Chlamydomonas reinhardtii) based on the HSR.⁸⁶ Moreover, another meaningful application of the HSR is that the seemingly hidden entropy production can be partially probed from the violation spectrum of FDR.⁸⁴ First of all, we state that both quantities can provide proper measures of deviation from equilibrium of many-body active particles. The difference is that in the

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experimental investigation, only the information of the spatial steadystate trajectories is required under our framework, while for HSR, the response spectrum and fluctuation spectrum of the system must be accessible. The amount of information contained in the violation spectrum determines how well the HSR probes the heat dissipation of the system. On the one hand, in small stochastic systems, it is a nontrivial task to directly measure the response functions, whereas details about spatial trajectories are easily observed. In fact, determining the response spectrum requires measuring each frequency separately, which must cover the high frequency region to ensure convergence of the integration in the HSR, substantially increasing the statistical effort.⁸⁷ On the other hand, to experimentally test the HSR, one needs to perturb the system. Conversely, our framework is noninvasive in experiments.

IV. ENTROPIC BOUNDS AND THERMODYNAMIC UNCERTAINTY RELATION(TUR)

According to Refs. 73 and 74, the entropic bounds on S_g , stronger than the second law, can be obtained by using the Cauchy–Schwarz inequality

$$\langle \dot{S}_g \rangle \le \langle \boldsymbol{D} \cdot (\boldsymbol{F}^{eff})^2 \rangle.$$
 (12)

This conclusion worthy of attention implies that the change rate of the generalized EP is bounded by an activity and configuration-dependent term. Actually, activity affects both sides of the equation, mainly through the activity dependent diffusivity D(x) and interaction $F^{eff}(x)$.

Now, we turn to an important universal inequality between the fluctuations in current and thermodynamic cost, the thermodynamic uncertainty relation (TUR).^{9–22,26,67} To see the TUR of ABPs, we consider a generalized current $\Theta[\chi]$ along a single trajectory χ defined as 26,73

$$\Theta[\chi] = \int \Lambda(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}} dt, \qquad (13)$$

where $\Lambda(\mathbf{x}) = (\Lambda_1(\mathbf{x}), \Lambda_2(\mathbf{x}), ..., \Lambda_N(\mathbf{x}))$ is a projection operator. Using different projection operator, one can get different kinds of current, such as the moving distance of particles or the EP in a time interval. The change rate of Θ can be written as

$$\langle \dot{\Theta} \rangle = \int \Lambda(\mathbf{x})^{\mathrm{T}} \mathbf{J}(\mathbf{x}, t) d\mathbf{x}.$$
 (14)

For instance, for the choice $\Lambda_i(\mathbf{x}) = \delta_{ik}$ in a steady state, the generalized observable current is the drift velocity of the kth active particle



FIG. 1. Validation of our key results, the TURs on the current $\Theta_1 = S_g$. Here, $B_1 = B(\Theta_1) = \frac{2\langle\Theta_1\rangle^2}{Var(\Theta_1)}$ measures the uncertainty of total entropy production and v_0 is the self-propelling velocity. We also plot the generalized entropy production $\langle\Delta S_g\rangle$, and the alternative entropy production $\langle\Delta S_g^{(1)}\rangle$ by treating the active system as an equilibrium system with a high effective temperature is also presented for comparison. Comparison between these quantities from the simulations has been presented for different values of the persistent time τ_p : $\tau_p = 0.0167$ (a), $\tau_p = 0.0333$ (b), $\tau_p = 0.0833$ (c), and $\tau_p = 0.167$ (d).

and $\Psi_i(\mathbf{x}) = \delta_{ik} D_i(\mathbf{x})$ only depends on the current configuration of the system.

Due to the markovity of effective dynamics, one can obtain¹⁶

$$\frac{Var[\Theta]}{\langle \Theta \rangle^2} \ge \frac{2}{\langle \Delta S_g \rangle},\tag{15}$$

which serves as a TUR for currents based on information of particleposition trajectories in the steady states. The effect of particle activity is reflected in the activity-dependent total EP $\langle \Delta S_g \rangle$. Mathematically, we have approximated the colored noise by a white one and obtained the effective Fokker-Planck equation, which facilitates following derivation. Only through this mapping, can we then set up a TUR, which can be numerically checked for real systems or even by experiments. Several notable points are presented as follows. First, in a steady state, the change in system entropy vanishes and, thus, $\langle \Delta S_g \rangle = \langle \Sigma_g \rangle / T$ $=T^{-1}\langle \int_{0}^{t_{f}}F^{eff}(\boldsymbol{x})^{\mathrm{T}}\circ\dot{\boldsymbol{x}}dt\rangle$. Second, the TUR $\langle\Delta S_{g}\rangle\geq 2\langle\Theta\rangle^{2}/Var[\Theta]$ gives the lower bound, and the entropic bound $\langle \dot{S}_{q} \rangle \leq \langle D \cdot (F^{eff})^{2} \rangle$ provides the upper bound of the generalized EP. Furthermore, as the generalized EP will decrease after coarse-grained approximation, Eq. (15) can even be used to infer the exact EP including the self-propulsion's contribution. Third, in Ref. 19, Tan Van Vu et al. indicated that the current fluctuation is constrained not only by the entropy production but also by the average dynamical activity in an athermal AOU model, by mathematically mapping the system into an underdamped one. As with the framework in most studies, the dynamic irreversibility measure that they define requires tracking the self-propelled velocities of active particles.

V. NUMERICAL RESULTS OF ABPs MODEL

In this part, we have discovered the generalized EP as well as the validity of entropic bound and TUR by direct numerical simulations. We consider a system with *N* disk-shaped particles in a twodimensional *xy* plane. Here, the exclusive-volume pair potentials of ABPs are modeled by the Weeks–Chandler–Anderson (WCA) potential: $U(r) = 4\epsilon [(\frac{d}{r})^{-12} - (\frac{d}{r})^{-6} + \frac{1}{4}]$ for $r < 2^{1/6}$, $\epsilon = k_B T$ and U=0. Here, $r = |\mathbf{x}_1 - \mathbf{x}_2|$ is the particle separation and ϵ is the interaction strength. Proper values of parameters have been chosen to illustrate our main results while N = 5120 throughout the paper. Here, we focus on the steady-state thermodynamics of the system, where the system entropy change vanishes. We need to emphasize that the thermodynamic quantities are obtained from the trajectories generating from Eqs. (1) and (2).

For a sufficiently large particle density ϕ , our numerical results show the MIPS: a coexistence between vapor and dense at a critical self-propulsion velocity $v_0^c(\phi)$, which is phase density dependent. To further demonstrate the phase separation, we introduce the local order parameter with respect to particle $i^{46,66}$

$$q^{6}(i) = \frac{1}{6} \left| \sum_{j \in N^{i}} \exp\left(i6\varphi_{ij}\right) \right|, \tag{16}$$

where N^i is the closest six neighboring particles of *i* and φ_{ij} is the angle between the bond vector connecting particle *i* to *j*.

A. TUR and entropic bound

To test the validity of TUR and entropic bound, we explore the ABPs model over $_0$, τ_p , and ϕ . In Fig. 1, we begin by choosing the current $\Theta_1 = S_g$ and plot the generalized EP $\langle \Delta S_g \rangle$ and $\langle \Delta S_g^{(1)} \rangle$ with the TUR bound $B_1 = B(\Theta_1) = 2\langle \Theta_1 \rangle^2 / Var[\Theta_1]$ over τ_p by varying $_0$. Indeed, one can see that all the data for B_1 lie below $\langle \Delta S_g \rangle$, demonstrating the validity of our TUR Eq. (15). Nevertheless, if one use $\langle \Delta S_g^{(1)} \rangle$ instead of $\langle \Delta S_g \rangle$, obvious violation presents while increasing the persistent time τ_p . Therefore, the simulation results clearly indicate that our method to treat the many-body ABPs system correctly establishes the TUR in a large range of persistence time τ_p .

In Fig. 2(a), we also plot how the generalized EP, $\langle \Delta S_g \rangle$ and $\langle \Delta S_g^{(1)} \rangle$, and TUR bound behave for different particle density ϕ . We find that the difference between $\langle \Delta S_g \rangle$ and $\langle \Delta S_g^{(1)} \rangle$ (normalized by the particles density) increases for larger ϕ . This means that the



FIG. 2. Further validation of the TURs and entropic bounds. (a) Comparison between the TUR bound $B_1 = B(\Theta_1) = 2\langle\Theta_1\rangle^2 / Var[\Theta_1]$, the generalized entropy production $\langle\Delta S_g\rangle$ and the alternative entropy production $\langle\Delta S_g^{(1)}\rangle$ (normalized by the particles density) for different particle density ϕ . Here, we choose $\Theta_1 = S_g$, $\tau_p = 0.0167$, and $v_0 = 50$. (b), (c) Numerical results of TURs of larger range τ_p . (b) Log ratio of the TUR parameter $\eta_g = \frac{2\langle\Theta|^2}{Var[\Theta|\langle\Delta S_g\rangle}$ and $\eta_g^{(1)} = \frac{2\langle\Theta|^2}{Var[\Theta|\langle\Delta S_g^{(1)}\rangle}$ for $v_0 = 50$ and $v_0 = 100$. When $\ln \eta \leq 0$, our TUR Eq. (15) is established, otherwise, the TUR is invalid. (c) The non-monotonic persistent time dependence of the generalized entropy production rate S_g when $v_0 = 50$. (d) Numerical validation of the entropic bound, Eq. (12), for a larger range of self-propelling velocity v_0 . Here, we choose $\tau_p = 0.0167$.

generalized EP S_g that we proposed may partially recover the information loss when simply treating the active particles system as an effective system with high temperature by considering the interparticle correlations at a coarse-grained level via Fox approximation. The difference between $\langle \Delta S_g \rangle$ and $\langle \Delta S_g^{(1)} \rangle$ becomes significant especially in a high density system.

Furthermore, in Fig. 2(b), we numerically calculate the TUR parameter $\eta_g = \frac{2\langle\Theta\rangle^2}{Var[\Theta]\langle\Delta S_g\rangle}$ and $\eta_g^{(1)} = \frac{2\langle\Theta\rangle^2}{Var[\Theta]\langle\Delta S_g^{(1)}\rangle}$ for a large range of τ_p when $v_0 = 50$ and $v_0 = 100$. If $\eta_g \leq 1$, our TUR Eq. (15) is established; otherwise, the TUR is invalid. The TUR still holds for a quite large $\tau_p = 10$, even though the Fox approximation might break down for such a large τ_p . Further increasing the value of τ_p , it can be observed that our TUR Eq. (15) also fails. In addition, we also plot the persistent time dependence of the generalized EP for larger range of τ_p in Fig. 2(c). More interestingly, we find that ΔS_g has a non-monotonic dependence on the persistence time, which is not consistent with the physical expectation that increasing the persistent time displaces the active particle systems progressively away from equilibrium. The non-monotonic persistence time dependence implies that the measure of dynamic irreversibility is not monotonically related to the degree of departure from equilibrium quantified by character of the effective equilibrium hypothesis necessarily.⁸⁹ In our opinion, this nontrivial phenomenon is mainly due to the fact that the coarsegrained method may not effectively restore the irreversibility of the system in large persistent-time regime. Actually, the establishment of the breakdown of the time-reversal symmetry for active systems with significant persistent motion is of great challenge. Thus, a deeper investigation of this disconnect is still an open question and deserves further investigation.

At last, we also validate the entropic bound Eq. (12) $\langle \hat{S}_g \rangle \leq \langle \mathbf{D} \cdot (\mathbf{F}^{eff})^2 \rangle$. In Fig. 2(d), we choose $\tau_p = 0.0167$ and the entropic bound has been numerically proved by varying the self-propelling velocity ₀.

B. Generalized entropy production and MIPS

Another fundamental question in the context of stochastic thermodynamics is whether entropy production/dynamical irreversibility can act as a tool for typifying phase transitions. Insight into this question has been gained in some recent studies.^{18,92–100} For instance, by analyzing the majority-vote model, Noa *et al.*⁹⁵ have argued that there are specific hallmarks of entropy production for a given transition, whether it is continuous or discontinuous.

We now focus on the relation between the dynamical irreversibility and MIPS in the ABPs system. The simulations are performed at a fixed particle density $\phi = 0.768$ by varying the velocity ₀, and the MIPS occurs at a critical value $v_0^c|_{\phi=0.768} \approx 54.3$. In Fig. 3(a), the steady-state generalized EPs, $\langle \Delta S_g \rangle$, have been shown. As ₀ increases, the systems are driven far away from equilibrium with $\langle \Delta S_g \rangle$ increasing. Furthermore, we find that the $\langle \Delta S_g \rangle - v_0$ derivative has inflection points and reaches the maximum near the phase transition point, providing the evidence that the generalized EP ΔS_g can be used to indicate the large scale MIPS. On the other hand, we also calculate the local entropy production (density), $\langle \Delta S_g^l(\mathbf{x}) \rangle$, by averaging the particles' entropy production in a local lattice around given position \mathbf{x} . As shown in Fig. 3(b), the local EP shows a strong contribution in the vicinity of



FIG. 3. (a) The generalized entropy production $\langle \Delta S_g \rangle$ and the corresponding first derivative have been plotted over the kinetic phases of MIPS. Here, the particles density $\phi = 0.768$ to guarantee the occurrence of MIPS. Vertical blue dashed dot lines indicate the critical velocity v_0^c . (b) Density and generalized entropy production $\langle \Delta S_g \rangle$ in a local lattice for ABPs model with MIPS have been plotted. Here, we choose $\phi = 0.768$ and $v_0 = 80 > v_0^c$. Vertical blue dashed dot lines indicate the interface of MIPS.

the interfaces between phases.⁶² In addition, we find that local entropy production almost vanishes in the high density phase due to the dynamical arrest effect.^{101,102} Thus, the coarse-grained entropy production ΔS_g also acts as a reliable measure to determine the boundary of MIPS. Finally, to investigate the connection between EP and defects, typical snapshots for $\phi = 0.768$ and $v_0 = 80 > v_0^c$ of the MIPS are shown in Fig. 4. Specifically, the structural information coded in the spatial distribution of the local order parameter for individual particles is shown in Fig. 4(a) with the generalized EP in Fig. 4(b) as a contrast. The defects are found to allow for the increase in the generalized EP of active particles. To confirm this conclusion clearly, we calculate the mean EP, $\langle \Delta S_g \rangle_a$, by averaging ΔS_g for all particles with same q^6 in a high density phase in Fig. 4(c). Clearly, the mean EP $\langle \Delta S_g \rangle_a$ decreases with the local order parameter q^6 increasing as expected.

VI. CONCLUSIONS

In conclusion, we focus on the thermodynamic quantities for active systems over a finite time interval in steady states. We establish the stochastic thermodynamics for the many-body active particle system based on an approximate FPE obtained via a time-local approximation. By mapping the systems into an equivalent Langevin equation, one can identify a generalized trajectory-dependent EP ΔS_g , wherein particle activity comes into play by a configuration-dependent diffusion coefficient and a many-body effective interaction force. The relationship between the generalized EP and the rich collective behaviors of active matter has been illustrated. Precisely, we utilize the generalized entropy production to identify the phase transition point, the interface and the defects in high density phases of MIPS, showing that the generalized EP acts as a tool to quantify the dynamical irreversibility on a macroscopic scale. Furthermore, the TUR and entropic bound for the currents in the steady state can be established successfully for a



FIG. 4. Snapshot configurations for $\phi = 0.768$ and $v_0 = 80 > v_0^c$ of the MIPS have been plotted: (a) local order parameter q^6 , (b) local entropy production $\langle \Delta S_g \rangle$ proposed by us. In Fig. 4(c), we show that the local entropy production $\langle \Delta S_g \rangle$ decreases for higher q^6 , which means that the entropy production of the particles in defects is larger.

large range of persistent time. In contrast, we show that simply mapping the system to an equivalent one with an effective temperature does not capture the right bounds, highlighting the suitable coarsegrained approach via Fox approximation. Due to the link between TURs and anomalous diffusion,¹⁰³ our results may help to bound the timescale of anomalous kinetics in active systems. We believe that our work can provide a deeper understanding of the stochastic thermodynamics in the many-body active particles system.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Science and Technology of China (MOST) (No. 2018YFA0208702) and National Science Foundation of China (Nos. 32090044, 21973085, 21833007, and 21790350).

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Z.-Y.C. and J.S. contributed equally to this work.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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