Thermodynamic uncertainty relation for active particle systems

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Understanding stochastic thermodynamics of active matter 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 dissipation cost, has not been established yet. Here, we address such an issue in a general model of active particle system by introducing an effective Fokker-Planck equation, which allows us to identify a generalized total entropy production along a stochastic trajectory, wherein an activity and configuration dependent diffusion coefficient comes into play with an important role. In this framework, we are able to derive the entropy bound as well as TUR associated with any generalized current in the system. Finally, we demonstrate the validity of our theoretical results by direct numerical simulations.

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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 system, fluctuations are significant, so that thermodynamic quantities become stochastic variables. This observation allows ones to generalize laws of thermodynamics on 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 fluctuations in current and thermodynamic cost, the thermodynamic uncertainty relation (TUR), has been discovered [9–21]. Specifically, TURs constrain the Fano factor of an arbitrary observable current by the total entropy production, indicating that the output in the process of thermodynamic dissipation will inevitably generate energy costs, and provide an alternative method to obtain a lower bound on the entropy production. Moreover, TURs make an irreplaceable contribution to our understanding of nonequilibrium phenomena (e.g., work extraction under measurement and feedback [18, 19, 22] and biological clocks [23]) which can provide more detailed information about the system than the second law. TUR was first proposed for biomolecular processes by Barato and Seifert [9] and then extended to many other situations, such as diffusion process [11, 12], finite-time generalization [11, 12, 16], periodically driven systems [14, 20], biological oscillators [17, 21, 24], time-delayed systems [25], etc. Very recently, the frontiers of stochastic thermodynamics have shifted to the study of active particle systems. The study of active particles is very helpful in understanding the behaviors of many biological systems [26–34] and of remarkable potentials in the design of synthetic colloidal systems with controllable properties. So far, the laws of thermodynamics, the definition of related entropy production or the construction of fluctuation theorem in active particle systems [35–46] has been discussed in a few studies. However, the ability of active particle systems completely altering the dynamical behaviors of interacting motile particles by consuming energy supplied internally or externally proposes a great challenge for establishing TUR in such systems.

In this letter, we address such an issue in the general AOU-T model [47] for active particles systems, wherein the self-propulsion force is realized by a colored noise described by the Ornstein-Uhlenbeck process , and thermal noise is present. Our starting point is an effective Fokker-Planck equation (FPE) governing the distribution function of particle positions, from which we can identify the trajectory-based total entropy production S_g, wherein a configuration dependent effective diffusivity plays an important role. The validity of FPE insures that $\langle \dot{S}_g \rangle \geq 0$ which can be interpretated as the second law in this active system. In addition, for any nonzero generalized current Θ, a stronger entropic bound for $\langle \dot{S}_g \rangle$ can be obtained in associated with $\langle \Theta \rangle$. Finally, a TUR between the variance of current $Var[\Theta]$ and total entropy production ΔS_g along a trajectory is well established as $Var[\Theta]/\langle \Theta \rangle^2 \geq 2/\langle \Delta S_g \rangle$. We validate these relations in a simple system with periodic potential, demonstrating that incorporation of activity into S_g is crucial to setup the right boundaries.

Model: We consider a homogeneous system of N active particles with spatial coordinate $\boldsymbol{x}(t) = \{x_1(t), \ldots, x_N(t)\}^T$. The particles move in a viscous medium and hydrodynamic interactions are neglected. The system dynamics is described by the following overdamped equation,

$$\dot{\boldsymbol{x}}(t) = \mu \boldsymbol{F}(\boldsymbol{x}, t) + \boldsymbol{\xi}(t) + \boldsymbol{\eta}(t). \tag{1}$$

Here $\boldsymbol{F}$ is the total force, μ is the mobility, $\boldsymbol{\xi}(t)$ is a Gaussian distributed thermal noise with zero mean and time correlation $\langle \xi_i(t)\xi_j(s) \rangle = 2D_t \delta_{ij} \delta(t-s)$. The translational diffusion coefficient D_t satisfies $D_t = \mu k_B T$ with k_B the Boltzmann constant (which is set to be 1 throughout the paper) and T the ambient temperature. The term $\boldsymbol{\eta}(t)$ represents the OU active components with zero

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mean and time correlation

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

wherein τ_p is the persistence time and v_0 denotes the self-propulsion speed [29, 30, 33, 48–50]. 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 $D_t + D_a$.

Effective FPE: Following the scheme proposed by Seifert [2], one can define the entropy production of the system along a given stochastic trajectory $\chi(t) = \{\boldsymbol{x}(t)|_{t=0}^{t=t_f}\}$ as $S_{sys}(t) = -\ln P(\boldsymbol{x},t)$, where $P(\boldsymbol{x},t)$ is the configurational probability distribution for the state variable to take the value $\boldsymbol{x}$ at time t. Since the AOU-T model (Eq.(1)) is non-Markovian, it is not possible to obtain an exact FPE for $P(\boldsymbol{x},t)$. To proceed, we adopt the Fox method [47, 51, 52] to get an effective FPE which can best approximate the process of physical interests and make accurate predictions [53–55] (see Appendix A for details), which reads

$$\partial_t P(\boldsymbol{x},t) = -\sum_{i=1}^{N} \partial_{x_i} J_i(\boldsymbol{x},t). \tag{3}$$

The probability current is given by

$$J_i(\boldsymbol{x},t) = D_i(\boldsymbol{x})\beta F_i^{eff}(\boldsymbol{x})P(\boldsymbol{x},t) - D_i(\boldsymbol{x})\partial_{x_i}P(\boldsymbol{x},t), \tag{4}$$

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

$$D_i(\boldsymbol{x}) = D_t + D_a\left[1 - \beta\tau\partial_{x_i}F_i(\boldsymbol{x})\right]^{-1} \tag{5}$$

with $\tau = \tau_p D_t/d^2$ a dimensionless persistence time. $F_i^{eff}(\boldsymbol{x}) = D_i^{-1}(\boldsymbol{x})[D_t F_i(\boldsymbol{x}) - T\partial_{x_i}D_i(\boldsymbol{x})]$ gives the effective force exerting on the i-th particle. For a passive system in the absence of $\boldsymbol{\eta}(t)$, $D_i(\boldsymbol{x}) = D_t$ and $F_i^{eff}(\boldsymbol{x}) = F_i(\boldsymbol{x})$, while in the limit $\tau_p \to 0$, $D_i(\boldsymbol{x}) = D_t + D_a$ and $F_i^{eff}(\boldsymbol{x}) = D_t F_i(\boldsymbol{x})/D_a$. Note that the Fox approximation is valid for $1 - \beta\tau\partial_i F_i(x) > 0$ such that $D_i(x)$ is positive in the entire area. This condition may break down when phase separation takes place in the system. Nevertheless, for the study of stochastic thermodynamics in the present work, one usually considers a nonequilibrium steady state where phase separation is not going to happen.

The Second Law: One notes that Eq.(3) corresponds to an equivalent Langevin equation. According to Sekimoto's suggestion [1], we can define generalized heat dissipation in the medium along a stochastic path $\chi(t)$ as

$$\Sigma[\chi] = \int_0^{t_f} \boldsymbol{F}^{eff}(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}}dt, \tag{6}$$

where "∘" stands for the Stratonovich product and the superscript 'T' means transposition. Since the effective force $\boldsymbol{F}^{eff}(\boldsymbol{x})$ is the total force done on the system including the effect of activity, the generalized heat dissipation will recover to the normal heat dissipation $\int_0^{t_f} \boldsymbol{F}(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}}dt$ in passive systems [2]. The difference between these two types of heat dissipations is the activity-induced extra entropy flux.

According to the Eq.(3), the change rate of the system entropy is

$$\begin{aligned}
\dot{S}_{sys}(t) &= -\partial_t \ln P(\boldsymbol{x},t) \\
&= -\frac{1}{P(\boldsymbol{x},t)}\Big[\frac{\partial P(\boldsymbol{x},t)}{\partial t} + \sum_{i=1}^{N} \partial_{x_i} P(\boldsymbol{x},t)|_{\boldsymbol{x}(t)}\dot{x}_i\Big] \\
&= -\frac{1}{P(\boldsymbol{x},t)}\Big[\frac{\partial P(\boldsymbol{x},t)}{\partial t} - \sum_{i=1}^{N} \frac{J_i(\boldsymbol{x},t)}{D_i(\boldsymbol{x})}|_{\boldsymbol{x}(t)}\dot{x}_i\Big] \\
&\quad - \beta\boldsymbol{F}^{eff}(\boldsymbol{x})^{\mathrm{T}}\dot{\boldsymbol{x}}.
\end{aligned} \tag{7}$$

Clearly, the final term in the third equality is related to the generalized heat dissipation in Eq.(6), i.e., $\beta\boldsymbol{F}^{eff}(\boldsymbol{x})^{\mathrm{T}}\dot{\boldsymbol{x}} = \dot{\Sigma}/T$. Then, Eq.(7) can be rewritten as a balance equation for the trajectory-dependent total entropy production

$$\dot{S}_g(t) = -\frac{\partial_t P(\boldsymbol{x},t)}{P(x,t)}|_{\boldsymbol{x}(t)} - \sum_{i=1}^{N} \frac{J_i(\boldsymbol{x},t)}{D_i(\boldsymbol{x})P(x,t)}|_{\boldsymbol{x}(t)}\dot{x}_i. \tag{8}$$

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

$$\langle \dot{S}_g(t)\rangle = \sum_{i=1}^{N} \int \frac{J_i(\boldsymbol{x},t)^2}{D_i(\boldsymbol{x})P(\boldsymbol{x},t)} d\boldsymbol{x} \geq 0, \tag{9}$$

where $\int d\boldsymbol{x}\partial_t P(\boldsymbol{x},t) = 0$ and $\langle \dot{x}_i|\boldsymbol{x},t\rangle = J_i(\boldsymbol{x},t)/P(\boldsymbol{x},t)$ have been used. Eq.(9) can be viewed as *the second law* of the active system, stating that the averaged total entropy production never decreases. All the information about particle activity is contained in $D_i(\boldsymbol{x})$ and $J_i(\boldsymbol{x})$.

Entropy bound on currents: The second law (Eq.(9)) ensures that the averaged total entropy production must increase with time. The equality holds if all the currents $J_i(x)$ vanish, i.e., the system can be mapped to an equivalent equilibrium system. If the system is in a steady state with nonvanishing current, which is often the case for the active particle system considered here, there could be stronger bounds on $\dot{S}_g$.

To see this, we consider a generalized current $\Theta[\chi]$ along a single trajectory χ defined as [25, 56]

$$\Theta[\chi] = \int \boldsymbol{\Lambda}(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}}dt, \tag{10}$$

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

$$\langle\dot{\Theta}\rangle = \int \boldsymbol{\Lambda}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{J}(\boldsymbol{x},t)d\boldsymbol{x}. \tag{11}$$

It can be proved by using Cauchy-Bunyakovsky-Schwarz inequality in a few lines (see Appendix B for details) that

$$\langle \dot{S}_g \rangle \geq \langle \dot{\Theta} \rangle^2 / |\boldsymbol{\Psi}|, \tag{12}$$

where $\boldsymbol{\Psi}(\boldsymbol{x})$ is a vector with $\Psi_i(\boldsymbol{x}) = D_i(\boldsymbol{x})\Lambda_i^2(\boldsymbol{x})$, and $|\cdot|$ represents the norm of the vector.

Eq. (12) constitutes the first main result in our paper. This conclusion worthy of attention implies that the change rate of the generalized total entropy production is bounded by every contribution to a generalized current in the system. Namely, any heat current is accompanied by a minimal rate of entropy production, offering a non-zero bound on entropy production rate which reveals more essential information of the system than the second law. Note that activity affects both sides of the equation, mainly through the configuration and activity dependent diffusivity $D_i(\boldsymbol{x})$.

Thermodynamic Uncertainty Relation(TUR): We now turn to investigate the TUR associated with the Fano factor of the current $\mathcal{F}(\Theta) = Var[\Theta]/\langle \Theta \rangle^2$ in the nonequilibrium steady state, where $Var[\Theta]$ stands for the variance of the current Θ. To this end, we consider a stochastic trajectory χ in time interval $(0, t_f)$ and introduce the scaled cumulant generating function

$$g(k, \Theta) = \ln \langle e^{k\Theta[x]} \rangle, \tag{13}$$

where k is a parameter. The expansion of $g(k, \Theta)$ in k contains terms with $Var[\Theta]$ and Θ, such that the investigation of this generating function can help us to get the bound on $\mathcal{F}(\Theta)$. Technically, one can introduce a supplemental force $\boldsymbol{f}(\boldsymbol{x}) = \alpha k \frac{\boldsymbol{J}^{ss}(\boldsymbol{x})}{P^{ss}(\boldsymbol{x})}$ into the system, where α is a variational parameter, so that an inequality of $g(k, \Theta)$ can be obtained as (see Appendix C for details)

$$\begin{aligned} g(k, \Theta) &\geq k \langle \int_0^{t_f} \dot{\Theta} dt \rangle^f - \frac{1}{4} \langle \int_0^{t_f} \boldsymbol{f} \boldsymbol{D}^{-1} \boldsymbol{f} dt \rangle^f \\ &= (1 + \alpha k) k \langle \Theta \rangle - \frac{1}{4} (\alpha k)^2 \langle \Delta S_g \rangle \end{aligned} \tag{14}$$

where $\langle \cdot \rangle^f$ denotes the average with respect to the solution of the modified system and

$$\langle \Theta \rangle = t_f \int \boldsymbol{\Lambda}(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{J}^{ss}(\boldsymbol{x}) d\boldsymbol{x} \tag{15}$$

is the average current along the trajectory.

In particular, choosing $\alpha = 2\langle \Theta \rangle / \langle \Delta S_g \rangle$ which makes the right hand side of above inequality the largest, one has

$$g(k, \Theta) \geq k(\langle \Theta \rangle) + \frac{k^2 \langle \Theta \rangle^2}{\langle \Delta S_g \rangle}. \tag{16}$$

Expanding the cumulant generating function up to second order in k, one has $g(k, \Theta) = k \langle \Theta \rangle + \frac{1}{2} Var[\Theta] k^2 + \mathcal{O}(k^3)$. Consequently, taking the limit $k \to 0$, one can obtain

$$\frac{Var[\Theta]}{\langle \Theta \rangle^2} \geq \frac{2}{\langle \Delta S_g \rangle} \tag{17}$$

which serves as the TUR for current in the active system. Eq.(17) serves as the second main result of the present paper. The effect of particle activity is reflected in the activity-dependent total entropy production $\langle \Delta S_g \rangle$.

In a steady state, for numerical purpose, the change of system entropy $\langle \Delta S_{sys} \rangle$ is negligible compared to the total entropy change and thus $\langle \Delta S_g \rangle \simeq \langle \Sigma \rangle / T = T^{-1} \left\langle \int_0^{t_f} F^{eff}(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}} dt \right\rangle$. To highlight the effect of activity, it would be instructive to consider a comparative case, where one can treat the active system as an equilibrium system with a high effective temperature $T_{eff} = \mu^{-1}(D_t + D_a)$, corresponding to the case in the limit $\tau_p \to 0$. Now the total entropy production is given by $\langle \Delta S_g^{(1)} \rangle = T_{eff}^{-1} \left\langle \int_0^{t_f} F(\boldsymbol{x})^{\mathrm{T}} \circ \dot{\boldsymbol{x}} dt \right\rangle$. To validate our main results Eq.(12) and Eq.(17), we can compare the bounds given by $\langle \Delta S_g \rangle$ to those given by $\langle \Delta S_g^{(1)} \rangle$, as will be done in following parts.

Numerical results and discussion: In this part, we would like to check the validity of the entropy bounds as well as TUR by direct numerical simulations. For simplicity but without lose of generality, we consider an active particle in a one-dimensional periodic potential subjected to a time-dependent external field, i.e., $F(x, t) = a \cos \omega x + \sin t$ with a a constant. The system is defined on a segment [0, 1] with periodic boundary conditions. The configuration dependent diffusion coefficient is given by $D(x) = D_t + D_a (1 + \beta \tau a \omega \sin \omega x)^{-1}$ and the effective force is given by

$$F^{eff}(x) = \frac{D_t}{D(x)} F(x) + \frac{a T \omega^2 \beta \tau D_a \cos \omega x}{D(x)(1 + \beta \tau a \omega \sin \omega x)^2}. \tag{18}$$

For illustration, we set $D_t = 0.05$, $a = 8$, $\omega = \pi/2$ and numerically solve Eq.(1) with time step $\Delta t = 0.001$ which is small enough. We collect 10^8 realizations to get the total entropy production and the moments of the current within time interval $t \in (0, 1)$. Three different types of currents are considered, namely $\Lambda_1(x) = 1$, $\Lambda_2(x) = x$ and $\Lambda_3(x) = \sin x$. Fig.1(a) shows the dependences of $E(\Theta) = \langle \Theta \rangle^2 / Var[\Theta]$ on time interval for persistence time $\tau_p = 0.1$(The results for other values of τ_p are qualitatively the same). Also shown are the total entropy production $\langle \Delta S_g \rangle$, and the one for comparison, saying $\langle \Delta S_g^{(1)} \rangle$. For the TUR to hold, one must have $E[\Theta] \leq \langle \Delta S_g \rangle / 2$. Indeed, one can see that all the data for $E[\Theta]$ lie below $\langle \Delta S_g \rangle / 2$, demonstrating the validity of our TUR Eq.(17). Nevertheless, if one use $\langle \Delta S_g^{(1)} \rangle$ instead of $\langle \Delta S_g \rangle$, obvious violation presents in the short observation time range. For the same consideration, we also do simulations to test and verify the entropic bounds on current. As shown in Fig.1(b), for different choices of τ_p, both the change rate of the generalized entropy production $\langle \dot{S}_g \rangle$ and the bound of currents given by $\langle \dot{\Theta} \rangle^2 / \langle D(x) \Lambda^2(x) \rangle$ vary monotonically. One can readily observe that $\langle \dot{S}_g \rangle$ is above all the bounds for all the τ_ps considered, demonstrating the validity given by Eq.(12). Nevertheless, if one uses $\langle \dot{S}_g^{(1)} \rangle$ instead of $\langle \dot{S}_g \rangle$, i.e., using the effective temperature scenario, it will be clearly

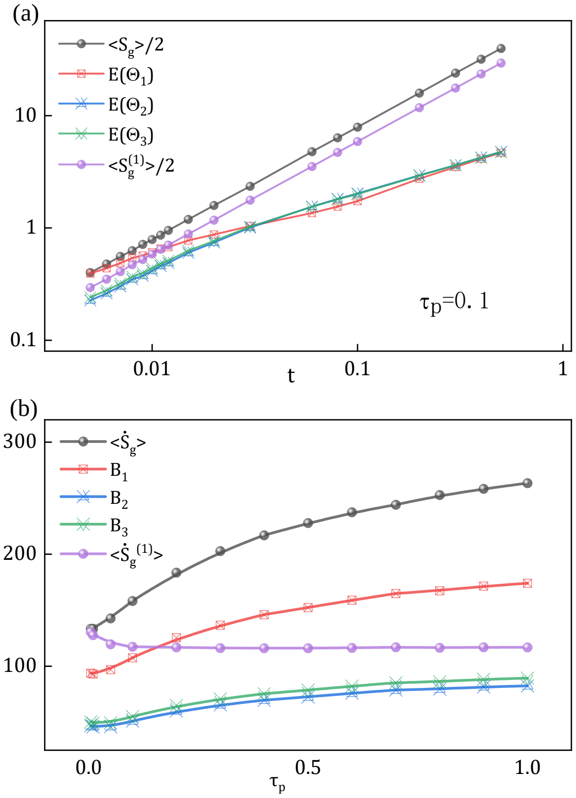

FIG. 1: Validation of our two key results, (a) the thermodynamic uncertainty relation and (b) entropic bounds on three different kinds of currents $\Theta_i (i = 1, 2, 3)$ whose projection operators are 1, x and $\sin(x)$ (x is the particle position), respectively. In (a), $\langle \Delta S_g \rangle/2$ is the generalized total entropy change, $E(\Theta_i) = \langle \Theta_i \rangle^2 / Var[\Theta_i] (i = 1, 2, 3)$ measures the uncertainty of total entropy production, t is the sampling time t, and τ_p is the persistent time. An alternative entropy production $\langle \Delta S_g^{(1)} \rangle/2$ by treating the active system as an equilibrium system with a high effective temperature is also presented for comparison. In (b), $\langle \dot{S}_g \rangle$ is the change rate of the generalized total entropy production, B_is are entropic bounds on Θ_is, respectively, and $\langle \dot{S}_g^{(1)} \rangle$ is the change rate of the alternative entropy production in the same effective equilibrium system as in (a).

smaller than the current bounds for $\Lambda_1 (\boldsymbol{x})$ if τ_p is larger than some value as shown in Fig.1(b), thus violating that bound condition for entropy production. Therefore, the simulation results clearly vindicate that our method to treat active particle systems correctly establishes the entropy bound and TUR in a large range of persistence time τ_p.

Actually, in general, active particle constitutes a new class of condensed matter systems that are inherently out of equilibrium, thus brings complexity to establish a theoretical framework for stochastic thermodynamics. Here, when studying the TUR, we focus on the evolution of the thermodynamic quantities for the system over a finite observation time interval. Under such a premise, the displacement of the active particles can be assimilated to a Markov process to some extent by making a time-local approximation. As presented in many works, mapping an active system to a passive equilibrium system with modified interaction potential and an approximate FPE has been successful in describing its large scale physics and dynamical properties [47, 53–55]. Here, we show that such a method can produce valuable insight into the stochastic thermodynamics of active particle systems.

Conclusion: In this letter, we proposed a theoretical framework to establish stochastic thermodynamics for a general active particle system based on an effective FPE obtained via Fox approximation. Special attentions were paid on the TUR and entropic bounds on currents. By mapping the system to an equivalent Langevin equation, one can identify a generalized trajectory-dependent entropy, wherein particle activity comes into play by a configuration and activity-dependent diffusion coefficient and a many-body effective interaction force. Within this framework, we are able to derive a bound for the change rate of the total entropy production associated with any generalized current in the system. In addition, the TUR for the current in the steady state can be established successfully. Direct numerical simulations demonstrate the validity of our theoretical results with varying system parameters such as the persistence time of the active force. In addition, we show that simply mapping the system to an equivalent one with an effective temperature does not capture the right bounds. We believe that our work can provide energetic insights and open new perspectives on stochastic thermodynamics in active systems.

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