

## Macroscopic time-reversal symmetry breaking at a nonequilibrium phase transition

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We study the entropy production in a globally coupled Brownian particles system that undergoes an order-disorder phase transition. Entropy production is a characteristic feature of nonequilibrium dynamics with broken detailed balance. We find that the entropy production rate is subextensive in the disordered phase and extensive in the ordered phase. It is found that the entropy production rate per particle vanishes in the disordered phase and becomes positive in the ordered phase following critical scaling laws. We derive the scaling relations for associated critical exponents. The disordered phase exemplifies a case where the entropy production is subextensive with the broken detailed balance.

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Detailed balance is the hallmark of the thermal equilibrium state. A system is said to obey detailed balance if the probability current along any microscopic trajectory in the phase space is balanced by that along the time-reversed one [1]. Consequently time-reversal symmetry is preserved in thermal equilibrium.

Thermodynamics of nonequilibrium systems, where detailed balance and time-reversal symmetry are broken and the total entropy production is positive by dissipating the housekeeping and excess heats, has been attracting much interest [2–10]. Recent studies have been focused on microscopic systems with a few degrees of freedom where the effect of thermal fluctuations are strong. Under the framework of stochastic thermodynamics, various fluctuation theorems are discovered, which provide useful insights on the nature of nonequilibrium fluctuations. Theoretical works foster experimental studies of microscopic systems such as molecular motors, nano heat engines, biomolecules, and so on [11–16].

Macroscopic systems pose an intriguing question on the level of irreversibility. Consider a many-particle system displaying an order-disorder phase transition whose microscopic dynamics does not obey detailed balance. Does the broken detailed balance result in time-reversal symmetry breaking at the macroscopic level? On the one hand, one may expect that entropy productions of each particle add up to a macroscopic amount irrespective of a macroscopic state. On the other hand, if the system is in a disordered phase so that all configurations are almost equally likely, then irreversibility may not show up on a macroscopic level producing only a subextensive amount of entropy. This question lead us to the study of the entropy production in a model system undergoing nonequilibrium phase transition.

In this paper, we investigate the emergence of macroscopic irreversibility out of microscopic dynamics with broken detailed balance. We find that the total entropy production changes its character from being subextensive to being extensive as the system undergoes an order-disorder phase transition. The entropy production rate per particle exhibits critical scaling laws as an order parameter does in ordinary critical phenomena, and scaling relations among critical exponents are derived. Although the results are derived in

a specific model system, we argue that the scaling behaviors should be valid for general nonequilibrium systems.

As a nonequilibrium model, we adopt a particle system which displays a collective motion. In nature a flock of birds and a school of fish display a collective motion [17–26]. Such a phenomenon has been studied with microscopic models consisting of active self-propelled particles moving at a constant speed [17–20,20,21]. Flocking takes place when particles are subject to an interaction that favors mutual alignment of velocities. These systems undergo nonequilibrium phase transition from a disordered phase to an ordered flocking phase as the interaction strength increases. Theoretical efforts have been devoted to understanding the mechanism leading to the flocking and the nature of the phase transition [17,20]. In this work, we focus on a Langevin system introduced in Ref. [27]. In comparison with the previous models with active particles, particles in this model are driven by the thermal noise in addition to the velocity aligning force. Thus, it allows us to study the thermodynamic quantities such as the entropy production.

The model in Ref. [27] is composed of passive particles in the thermal reservoir instead of active particles. It consists of  $N$  Brownian particles of mass  $m$  in a two-dimensional plane of size  $L \times L$  embedded in a thermal reservoir at constant temperature  $T$ . The particle density is denoted by  $\rho = N/L^2$ . Let  $\mathbf{x}_i = (x_{i1}, x_{i2})$  and  $\mathbf{v}_i = \frac{d\mathbf{x}_i}{dt} = (v_{i1}, v_{i2})$  be the position and the velocity of a particle  $i = 1, \dots, N$ . We will represent a configuration of the whole system with a shorthand notation  $\mathbf{Z} = (\mathbf{X}, \mathbf{V})$  with  $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$  and  $\mathbf{V} = \{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N\}$ . The equations of motion are given by

$$m \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i(\mathbf{V}) - \gamma \mathbf{v}_i + \boldsymbol{\xi}_i(t), \quad (1)$$

where  $\gamma$  is the damping coefficient and  $\boldsymbol{\xi}_i(t) = (\xi_{i1}(t), \xi_{i2}(t))$  is the thermal noise satisfying

$$\begin{aligned} \langle \xi_{ia}(t) \rangle &= 0, \\ \langle \xi_{ia}(t) \xi_{jb}(t') \rangle &= 2\gamma k_B T \delta_{ij} \delta_{ab} \delta(t - t') \end{aligned} \quad (2)$$

with the Boltzmann constant  $k_B$ , which will be set to unity hereafter. The velocity aligning force  $\mathbf{F}_i(\mathbf{V})$  is taken to be

$$\mathbf{F}_i(\mathbf{V}) = \Gamma \hat{\mathbf{v}}_i \times (\mathbf{f} \times \hat{\mathbf{v}}_i) = \Gamma [\mathbf{f} - (\mathbf{f} \cdot \hat{\mathbf{v}}_i) \hat{\mathbf{v}}_i], \quad (3)$$

where  $\Gamma$  is the interaction strength,  $\hat{\mathbf{v}}_i = \mathbf{v}_i/|\mathbf{v}_i|$  is the unit vector, and

$$\mathbf{f} = \frac{1}{N} \sum_{j=1}^N \hat{\mathbf{v}}_j. \quad (4)$$

The vector  $\mathbf{f}$  points towards the average direction of the particles, and its magnitude  $\Lambda = |\mathbf{f}|$  plays a role of the order parameter for the collective motion. Note that the force  $\mathbf{F}_i$  is perpendicular to  $\mathbf{v}_i$ . It does not work on the particle but turns the direction of  $\mathbf{v}_i$  toward  $\mathbf{f}$ . The interaction is infinite-ranged. A short-ranged version of the model was studied in Ref. [28].

Numerical study in Ref. [27] found that the system undergoes a phase transition separating a disordered phase ( $\Gamma < \Gamma_c$ ) and an ordered phase ( $\Gamma > \Gamma_c$ ). Near  $\Gamma = \Gamma_c$ , the order parameter scales as  $\langle \Lambda \rangle_s \sim (\Gamma - \Gamma_c)^\beta$  and the fluctuation  $\chi \equiv N(\langle \Lambda^2 \rangle_s - \langle \Lambda \rangle_s^2)$  scales as  $\chi \sim |\Gamma - \Gamma_c|^{-\gamma}$ , where  $\langle \cdot \rangle_s$  denotes the steady-state ensemble average. The critical exponents are given by  $\beta/\nu \simeq 0.491$  and  $\gamma/\nu \simeq 1.02$ , where  $\nu \simeq 0.94$  is the correlation length exponent ( $\xi \sim |\Gamma - \Gamma_c|^{-\nu}$ ) [27]. These exponents are compatible with those of the mean field XY model [29,30]. When the interaction is infinite-ranged, the correlation volume  $\xi_V$  is more useful than the correlation length  $\xi$ . Since the model under consideration is embedded in the two-dimensional space, the correlation volume is given by  $\xi_V = \xi^2$  and scales as  $\xi_V \sim |\Gamma - \Gamma_c|^{-\bar{\nu}}$  with  $\bar{\nu} = 2\nu$ .

The velocity-dependent force breaks the detailed balance and the time-reversal symmetry. We quantify the amount of the time-reversal symmetry breaking by the entropy production. Suppose that the system evolves along a stochastic trajectory  $\mathcal{Z}[\tau] = \{(X(t), V(t)) | 0 \leq t \leq \tau\}$  for a time interval  $\tau$ . Following stochastic thermodynamics [10], the total entropy production  $\Delta S_{\text{tot}}[\mathcal{Z}[\tau]]$  along a given trajectory  $\mathcal{Z}[\tau]$  is determined by the probability ratio of  $\mathcal{Z}[\tau]$  against its time-reversed trajectory  $\mathcal{Z}^R[\tau] = \{(X(\tau - t), -V(\tau - t)) | 0 \leq t \leq \tau\}$  [10,31–35].

In our model, the total entropy production is decomposed into three terms as (see Appendix A)

$$\Delta S_{\text{tot}}[\mathcal{Z}] = \Delta S_{\text{sys}}[\mathcal{Z}] - \frac{Q[\mathcal{Z}]}{T} + \Delta S_v[\mathcal{Z}], \quad (5)$$

where  $\Delta S_{\text{sys}}$  is the change in the Shannon entropy of the system, and the second term is the Clausius form for the entropy change of the heat bath with  $Q$  being the heat absorbed by the system. The last term  $S_v$  appears only in the presence of a velocity-dependent force [35] and is given by

$$\Delta S_v[\mathcal{Z}] = \frac{m}{\gamma T} \sum_{i=1}^N \int_0^\tau dt \mathbf{F}_i(\mathbf{V}(t)) \circ \frac{d\mathbf{v}_i(t)}{dt}. \quad (6)$$

In the steady state, the ensemble average of  $\Delta S_{\text{sys}}$  vanishes. The thermodynamic first law reads as  $\Delta E = Q + W$  where  $\Delta E$  is the change in the total energy  $E = \sum_i \frac{1}{2} m \mathbf{v}_i^2$  and  $W = \sum_i \int_0^t dt \mathbf{v}_i \cdot \mathbf{F}_i$  is the work done by the force. Since  $W = 0$ ,  $Q = \Delta E$  and its steady state average vanishes. Thus, the entropy production rate per particle in the steady state is given by

$$s \equiv \frac{1}{N} \left\langle \frac{dS_{\text{tot}}}{dt} \right\rangle_s = \frac{m}{\gamma T} \frac{1}{N} \sum_{i=1}^N \left\langle \mathbf{F}_i \circ \frac{d\mathbf{v}_i}{dt} \right\rangle_s. \quad (7)$$

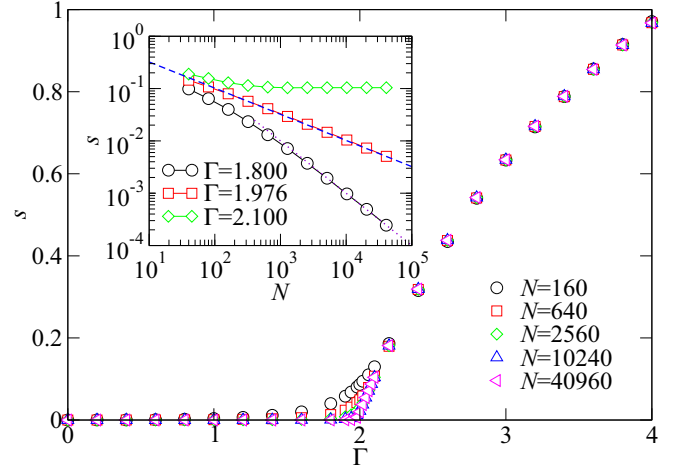


FIG. 1.  $s$  versus  $\Gamma$  for several values of  $N$ . Inset shows the finite size scaling behaviors of  $s$  when  $\Gamma$  is below, equal to, and above  $\Gamma_c = 1.976$ . The dotted (dashed) line has the slope  $-1$  ( $-1/2$ ).

This is the production rate of the housekeeping entropy that is necessary for maintaining the nonequilibrium steady state [5,9,31,32].

We have performed numerical simulations. The equations of motion in (1) are integrated numerically by using the time-discretized ( $\Delta t = 0.01$ ) Heun algorithm [36]. We took  $m = \gamma = \rho = 2T = 1$  in all simulations. Figure 1 shows that  $s$  displays a characteristic behavior signaling a continuous phase transition. As  $N$  increases,  $s \sim 1/N$  for  $\Gamma < \Gamma_c$  while it converges to a finite value for  $\Gamma > \Gamma_c$ . We also measure the fluctuation of the entropy production that is defined as

$$\chi_s(\Gamma, N, \tau) = \frac{1}{\tau N} \left[ \langle \Delta S_v^2 \rangle_s - \langle \Delta S_v \rangle_s^2 \right], \quad (8)$$

where  $\Delta S_v$  denotes the entropy production of  $N$  particles in a time interval  $\tau$ . Figure 2(a) shows the fluctuation measured at fixed  $\tau = 64$ . It has a sharp peak at  $\Gamma = \Gamma_c$ , which also reminds us of a continuous phase transition. The threshold  $\Gamma_c \simeq 1.976$  is close to the onset of the collective motion reported in

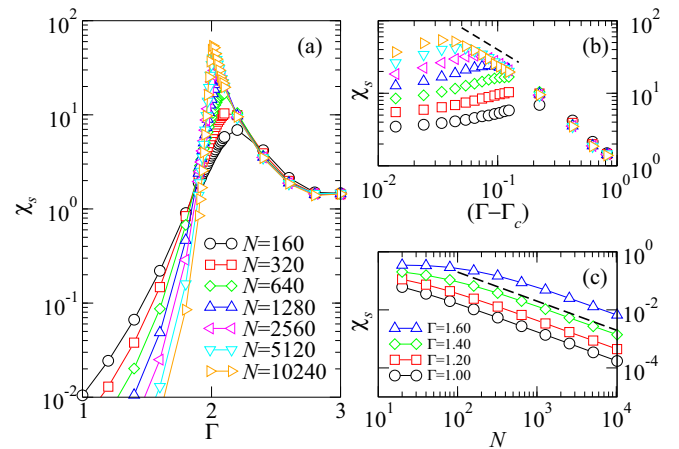


FIG. 2. (a) Fluctuation  $\chi_s$  as a function of  $\Gamma$ . (b)  $\chi_s$  versus  $(\Gamma - \Gamma_c)$  in the log-log scale. The dashed line has the slope  $-1$ . (c)  $\chi_s$  versus  $N$  for  $\Gamma < \Gamma_c$ . The dashed line has the slope  $-1$ .

Ref. [27]. We will show that the entropy production indeed exhibits the continuous phase transition and that the phase transition is triggered by the onset of the collective motion.

The entropy production can be related to the order parameter  $\Lambda$  for the collective motion. Using the equations of motion for  $d\mathbf{v}_i/dt$ , the entropy production in (6) is written as (see Appendix B)

$$\Delta S_v = \sum_{i=1}^N \int_0^\tau dt \left[ \frac{1}{\gamma T} |\mathbf{F}_i|^2 + \frac{1}{m} \nabla_{\mathbf{v}_i} \cdot \mathbf{F}_i \right] + \sum_{i=1}^N \frac{1}{\gamma T} \int_0^\tau \mathbf{F}_i \cdot d\mathbf{W}_i(t), \quad (9)$$

where  $\nabla_{\mathbf{v}_i}$  denotes the gradient operator with respect to  $\mathbf{v}_i$  and  $d\mathbf{W}_i(t) = \int_t^{t+dt} dt' \boldsymbol{\xi}_i(t')$ . The last term contributes neither to the ensemble average nor to the fluctuation because it is of the order of  $O(\tau^{1/2})$  with zero mean while the others scale linearly with  $\tau$ . Hence, it will be ignored. We then introduce the polar coordinate so that the velocity vector is written as  $\mathbf{v}_i = (v_i \cos \theta_i, v_i \sin \theta_i)$ . The relation (4) for the vector  $\mathbf{f} = (\Lambda \cos \psi, \Lambda \sin \psi)$  is written as

$$\Lambda e^{i\psi} = \frac{1}{N} \sum_{j=1}^N e^{i\theta_j}. \quad (10)$$

By using (3) and (10), we can show that (see Appendix B)

$$\Delta S_v = \sum_{i=1}^N \int_0^\tau dt [A_i - B_i + C_i] + O(\tau^{1/2}), \quad (11)$$

where  $A_i = \frac{\Gamma^2 \Lambda^2}{\gamma T} \sin^2(\psi - \theta_i)$ ,  $B_i = \frac{\Gamma \Lambda}{m v_i} \cos(\psi - \theta_i)$ , and  $C_i = \frac{\Gamma}{N m v_i}$ .

The expression in (11) gives a hint on the scaling behavior of the entropy production. The macroscopic variables  $\Lambda$  and  $\psi$  fluctuate much slower than the microscopic variables  $v_i$  and  $\theta_i$ . Thus, in taking the ensemble average of (11), we can use the adiabatic approximation [30] to replace  $\Lambda^2$  and  $\Lambda$  with their ensemble averaged values. Power counting combined with the adiabatic approximation leads to the conclusion that the entropy production rate per particle scales as  $s \sim \langle \Lambda^2 \rangle_s \sim \langle \Lambda \rangle_s^2$  (from  $A_i$  and  $B_i$ ) with the  $O(N^{-1})$  correction (from  $C_i$ ). Therefore, we expect that the entropy production rate per particle exhibits a critical power law scaling

$$s \sim (\Gamma - \Gamma_c)^{\beta_e} \quad (12)$$

with the critical exponent

$$\beta_e = 2\beta \quad (13)$$

for  $\Gamma > \Gamma_c$  and  $s \sim 1/N$  for  $\Gamma < \Gamma_c$ . When  $N$  is finite, following the standard finite-size-scaling (FSS) ansatz, we expect that

$$s = N^{-\beta_e/\bar{\nu}} \Phi[(\Gamma - \Gamma_c) N^{1/\bar{\nu}}]. \quad (14)$$

The scaling function  $\Phi(x)$  has the limiting behaviors  $\Phi(x) \xrightarrow{x \gg 1} x^{\beta_e}$  ensuring (12) and  $\Phi(x) \xrightarrow{x \ll -1} |x|^{\beta_e - \bar{\nu}}$  guaranteeing the  $N^{-1}$  scaling in the disordered phase.

The numerical data in Fig. 1 are analyzed according to the FSS form with the mean field critical exponents  $\beta_e = 1$  and

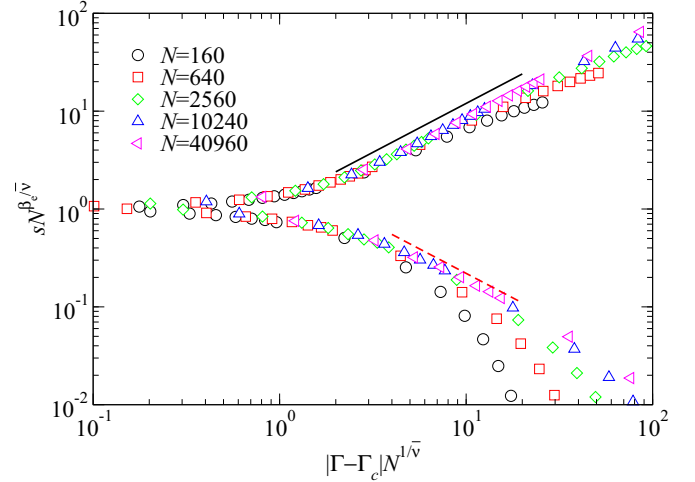


FIG. 3. Scaling plot of  $s N^{\beta_e/\bar{\nu}}$  versus  $|\Gamma - \Gamma_c| N^{1/\bar{\nu}}$  according to (14). The solid (dashed) line has slope 1(-1).

$\bar{\nu} = 2$ . As shown in Fig. 3, the data collapse and the limiting behaviors of the scaling function confirm the scaling relation in (13) and the FSS form of (14).

The total entropy production  $\Delta S_v$  is given by the spatial and temporal sum of the fluctuating local entropy production rates. We can derive the scaling form for the fluctuation  $\chi_s$  in the following way: Near the critical point, the correlation volume and time diverge as  $\xi_V \sim |\Gamma - \Gamma_c|^{-\bar{\nu}}$  and  $\xi_t \sim |\Gamma - \Gamma_c|^{-\nu_t}$ , respectively. When  $N \gg \xi_V$  and  $\tau \gg \xi_t$  in the ordered phase ( $\Gamma > \Gamma_c$ ), the total entropy production  $\Delta S_v$  is the sum of the contributions from  $M = \tau N / (\xi_t \xi_V)$  space-time blocks. All the blocks are independent because they are beyond the correlation volume and time. Therefore, the fluctuation should scale as  $\chi_s \sim \frac{1}{\tau N} \times M \times (\xi_t \xi_V s)^2 \sim \xi_t \xi_V s^2$ , which leads to the scaling form

$$\chi_s \sim (\Gamma - \Gamma_c)^{-\gamma_e} \quad (15)$$

with the exponent

$$\gamma_e = \nu_t + \bar{\nu} - 2\beta_e. \quad (16)$$

This is the hyperscaling relation extended to the systems with anisotropic scaling [37,38]. At the critical point, the finite-size effect dominates so that

$$\chi_s(\Gamma_c, N, \tau) \sim \begin{cases} \tau^{\gamma_e/\nu_t}, & \tau \ll N^{\bar{z}} \\ N^{\gamma_e/\bar{\nu}}, & \tau \gg N^{\bar{z}} \end{cases} \quad (17)$$

with  $\bar{z} = \nu_t/\bar{\nu}$ . In the disordered phase, the entropy production rate per particle vanishes as  $s \sim 1/N$ , so does the fluctuation  $\chi_s \sim 1/N$ .

The numerical data support the scaling theory. Figure 2(b) shows the fluctuation follows the power law of (15) with  $\gamma_e = 1$ . This exponent value satisfies the hyperscaling relation in (16) with  $\nu_t = 1$ ,  $\bar{\nu} = 2$ , and  $\beta_e = 1$ . The  $1/N$  scaling inside the disordered phase is also checked in Fig. 2(c). The FSS behavior at the critical point  $\Gamma = \Gamma_c$  is examined in Fig. 4. At a given  $N$ ,  $\chi_s(\Gamma_c, N, \tau)$  increases algebraically with  $\tau$  and saturates to a limiting value [see Fig. 4(a)]. The scaling plot in Fig. 4(b) confirms the scaling behavior of (17) for  $\tau \ll N^{\bar{z}}$  and  $\tau \gg N^{\bar{z}}$ .

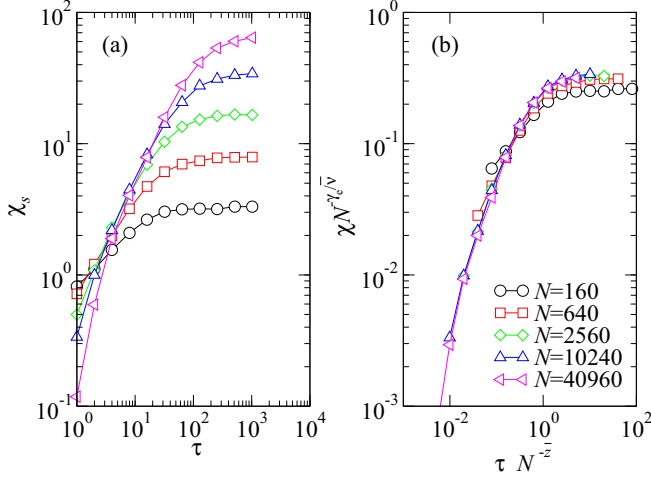


FIG. 4. (a)  $\chi_s(\Gamma_c, N, \tau)$  versus  $\tau$  at several values of  $N$ . (b) Scaling plot of  $\chi_s(\Gamma_c, N, \tau)N^{-\gamma_e/\nu}$  versus  $\tau N^{-z}$ .

We have shown that the broken detailed balance leads to the macroscopic entropy production only in the ordered phase using the analytic scaling theory and the numerical simulations. The entropy production per particle per unit time  $s$  is positive but vanishes as  $1/N$  in the disordered phase, while it is finite in the ordered phase following the power law [see (12)]. The fluctuation  $\chi_s$  vanishes in the disordered phase and follows the power law [see (15)] in the ordered phase. The critical exponents satisfy the scaling relations in (13) and (16).

The quadratic relation  $s \sim \langle \Lambda \rangle_s^2$  is crucial in deriving the scaling theory. This relation is derived in a model system that has a mean field nature. We argue that the scaling behaviors may be universal in general thermal systems undergoing a nonequilibrium phase transition between a near-equilibrium disordered phase and a nonequilibrium ordered phase. Collective motions in the ordered phase are characterized by the thermodynamic currents  $J_i$  of, e.g., energy and particle. The currents are small near the critical point. Thus, following the linear irreversible thermodynamics of Onsager [39], one can assume that  $J_i = \sum_j L_{ij} X_j$  where  $X_j$  are the thermodynamic forces and  $L_{ij}$  are the Onsager coefficients. The entropy production rate is then given by  $dS/dt = \sum_i X_i J_i = \sum_{i,j} L_{ij}^{-1} J_i J_j \propto J^2$ , which supports the validity of the quadratic relation between the entropy production rate and the current density. In stochastic thermodynamics, the total entropy production rate is written as the configuration space average of the probability current density squared [10], which also supports the relation. It would be interesting to investigate the scaling relations in (13) and (16) in systems with a short-ranged interaction.

The result that the ordered phase costs more environmental entropy production may be understood in the framework of the thermodynamic second law. Suppose that one changes a coupling constant of a system so that it relaxes from a disordered phase to an ordered phase in a characteristic relaxation time  $t_{\text{relax}}$ . During the process, the system entropy decreases at the rate  $dS_{\text{sys}}/dt \sim \Delta S_{\text{sys}}/t_{\text{relax}} = [S_{\text{sys}}(\text{ordered}) - S_{\text{sys}}(\text{disordered})]/t_{\text{relax}} < 0$ . The thermodynamic second law requires that the entropy production rate should be non-

negative at any moment. Therefore, during the relaxation process, the environmental entropy production rate should satisfy  $dS_{\text{env}}/dt \geq -dS_{\text{sys}}/dt \sim |\Delta S_{\text{sys}}|/t_{\text{relax}}$ , which gives a lower bound for the environmental entropy production rate. It should be investigated further whether the inequality is working in the steady state. We leave it for future work.

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## APPENDIX A: TOTAL ENTROPY PRODUCTION

It is straightforward to decide whether a deterministic dynamics is reversible or not. Suppose that a system evolves from a configuration  $Z(0) = (X(0), V(0))$  to  $Z(\tau) = (X(\tau), V(\tau))$  along a trajectory  $\mathcal{Z}[\tau] = \{Z(t) | 0 \leq t \leq \tau\}$ . If one flips the velocity in the final configuration and takes the resulting configuration  $(X(\tau), -V(\tau))$  as an initial state, then the reversible dynamics lets the system follow the time-reversed trajectory  $\mathcal{Z}^R[\tau] = \{Z^R(t) | 0 \leq t \leq \tau\}$  with  $Z^R(t) \equiv (X(\tau - t), -V(\tau - t))$ .

Generalizing this idea to stochastic systems, one can define the irreversibility or the entropy production by comparing the probability of trajectories  $\mathcal{Z}[\tau]$  and  $\mathcal{Z}^R[\tau]$ . The probability distribution function (PDF) of a given trajectory  $\mathcal{Z}[\tau]$  is given by  $P[\mathcal{Z}[\tau]] = \Pi[\mathcal{Z}[\tau]; Z(0)] p_0(Z(0))$ , where  $p_0(Z)$  is an initial PDF of being in a configuration  $Z$  at time  $t = 0$  and  $\Pi[\mathcal{Z}[\tau]; Z(0)]$  is a conditional probability distribution of  $\mathcal{Z}[\tau]$  to a given initial configuration  $Z(0)$ . The PDF for a time-reversed trajectory  $\mathcal{Z}^R[\tau]$  is similarly given by  $P[\mathcal{Z}^R[\tau]] = \Pi[\mathcal{Z}^R[\tau]; Z^R(0)] p_\tau(Z(\tau))$ , where  $p_\tau(Z)$  is the PDF at time  $\tau$  which has evolved from  $p_0(Z)$ . According to stochastic thermodynamics, the total entropy production for a given trajectory  $\mathcal{Z}[\tau]$  is given by [10]

$$\Delta S_{\text{tot}} = \ln \frac{\Pi[\mathcal{Z}[\tau]; Z(0)] p_0(Z(0))}{\Pi[\mathcal{Z}^R[\tau]; Z^R(0)] p_\tau(Z(\tau))}. \quad (\text{A1})$$

It consists of two parts as  $\Delta S_{\text{tot}} = \Delta S_{\text{sys}} + \Delta S_{\text{env}}$ , where

$$\Delta S_{\text{sys}} = -\ln p_\tau(Z(\tau)) + \ln p_0(Z(0)) \quad (\text{A2})$$

is the system entropy change and the remaining term  $\Delta S_{\text{env}}$  is the environmental entropy production.

The environmental entropy production can be written in terms of physical quantities. This task has been done in a recent preprint [35] for systems with an arbitrary velocity-dependent force. We make use of Eq. (11) of Ref. [35] to obtain that

$$\begin{aligned} \Delta S_{\text{env}} = & -\frac{m}{T} \sum_{i=1}^N \int_0^\tau \mathbf{v}_i(t) \circ d\mathbf{v}_i(t) \\ & + \frac{m}{\gamma T} \sum_{i=1}^N \int_0^\tau \mathbf{F}_i(\mathbf{V}(t)) \circ d\mathbf{v}_i(t), \end{aligned} \quad (\text{A3})$$

where the notation  $\mathbf{A}(t) \circ d\mathbf{B}(t) \equiv \frac{\mathbf{A}(t+d\mathbf{t}) + \mathbf{A}(t)}{2} \cdot [\mathbf{B}(t+d\mathbf{t}) - \mathbf{B}(t)]$  stands for the stochastic integral in the Stratonovich sense [1]. Using  $m d\mathbf{v}_i = (m d\mathbf{v}_i - \mathbf{F}_i dt) + \mathbf{F}_i dt$  in the first

term, one can further decompose  $\Delta S_{\text{env}}$  as

$$\begin{aligned} \Delta S_{\text{env}} = & -\frac{\sum_{i=1}^N \int_0^\tau \mathbf{v}_i \circ (m d\mathbf{v}_i - \mathbf{F}_i dt)}{T} \\ & -\frac{\sum_{i=1}^N \int_0^\tau \mathbf{v}_i \circ \mathbf{F}_i dt}{T} + \frac{m}{\gamma T} \sum_{i=1}^N \int_0^\tau \mathbf{F}_i(\mathbf{V}) \circ d\mathbf{v}_i. \end{aligned} \quad (\text{A4})$$

The Langevin equation indicates that

$$\begin{aligned} Q = & \sum_{i=1}^N \int_0^\tau \mathbf{v}_i \circ \left( m \frac{d\mathbf{v}_i}{dt} - \mathbf{F}_i \right) dt \\ = & \sum_{i=1}^N \int_0^\tau \mathbf{v}_i \circ (-\gamma \mathbf{v}_i + \boldsymbol{\xi}_i) dt \end{aligned} \quad (\text{A5})$$

is the work done by the heat bath through the damping force and the random force, namely the heat absorbed by the system from the heat bath. The second term is identically zero since  $\mathbf{v}_i \perp \mathbf{F}_i$ . The third term is  $\Delta S_v$ . This completes the derivation of Eqs. (5) and (6). In  $\Delta S_{\text{tot}}$ ,  $(\Delta S_{\text{sys}} - Q/T)$  is generic in all thermal systems, while the others appear only in the presence of velocity-dependent forces.

Note that the force  $\mathbf{F}_i$  does not work ( $W = 0$ ). Consequently, the thermodynamic first law is written as  $\Delta E = Q$ , where  $\Delta E$  is the change in the total kinetic energy  $E \equiv \sum_{i=1}^N \frac{1}{2} m \mathbf{v}_i^2$ .

## APPENDIX B: DERIVATION OF EQS. (9) AND (11)

The Stratonovich product  $\mathbf{F}_i \circ d\mathbf{v}_i$  is defined as [1]

$$\begin{aligned} \mathbf{F}_i \circ d\mathbf{v}_i = & \frac{\mathbf{F}_i(\mathbf{V}(t+dt)) + \mathbf{F}_i(\mathbf{V}(t))}{2} \cdot d\mathbf{v}_i(t) \\ = & \sum_a F_{ia}(t) dv_{ia} + \frac{1}{2} \sum_{j,a,b} \frac{\partial F_{ia}}{\partial v_{jb}} dv_{ia} dv_{jb} + o(dt), \end{aligned} \quad (\text{B1})$$

where  $i, j = 1, \dots, N$  are particle indices and  $a, b = 1, 2$  are Cartesian coordinate indices. We now use the Langevin equation to replace  $m d\mathbf{v}_i = \mathbf{F}_i dt - \gamma \mathbf{v}_i dt + d\mathbf{W}_i$ , where  $d\mathbf{W}_i = \int_t^{t+dt} dt' \boldsymbol{\xi}_i(t')$  satisfying that  $\langle dW_{ia} \rangle = 0$  and  $\langle dW_{ia} dW_{jb} \rangle =$

$2\gamma T \delta_{ij} \delta_{ab} dt$ . Inserting this into (B1), we obtain that

$$\begin{aligned} m \mathbf{F}_i \circ d\mathbf{v}_i = & |\mathbf{F}_i|^2 dt + \mathbf{F}_i \cdot d\mathbf{W}_i \\ & + \frac{1}{2m} \sum_{j,a,b} \frac{\partial F_{ia}}{\partial v_{jb}} dW_{ia} dW_{jb} + o(dt). \end{aligned} \quad (\text{B2})$$

Since  $dW_{ia}$  are independent of each other, one can replace  $(dW_{ia} dW_{jb})$  with  $(2\gamma T \delta_{ij} \delta_{ab} dt)$  [1]. This yields

$$\begin{aligned} \Delta S_v = & \sum_{i=1}^N \int_0^\tau dt \left[ \frac{1}{\gamma T} |\mathbf{F}_i|^2 + \frac{1}{m} \nabla_{\mathbf{v}_i} \cdot \mathbf{F}_i \right] \\ & + \frac{1}{\gamma T} \sum_{i=1}^N \int_0^\tau \mathbf{F}_i \cdot d\mathbf{W}_i, \end{aligned} \quad (\text{B3})$$

which is Eq. (9). As explained before, the last term can be neglected.

The expression for  $\Delta S_v$  becomes simpler in the polar coordinate. Let  $v_i$  and  $\theta_i$  are the magnitude and the polar angle of  $\mathbf{v}_i$ , respectively. The magnitude  $\Lambda$  and the polar angle  $\psi$  of  $\mathbf{f}$  are given by  $\Lambda e^{i\psi} = \frac{1}{N} \sum_j e^{i\theta_j}$ . The force  $\mathbf{F}_i = \Gamma(\mathbf{f} - (\mathbf{f} \cdot \hat{\mathbf{v}}_i) \hat{\mathbf{v}}_i)$  corresponds to the projection of  $\mathbf{f}$  in the normal direction of  $\mathbf{v}_i$ . Thus, one can write

$$\mathbf{F}_i = \Gamma \Lambda \sin(\psi - \theta_i) \hat{\boldsymbol{\theta}}_i, \quad (\text{B4})$$

where  $\hat{\boldsymbol{\theta}}_i$  is the unit vector in the polar angle direction of  $\mathbf{v}_i$ . It is evident that  $|\mathbf{F}_i| = \Gamma \Lambda |\sin(\psi - \theta_i)|$ . The divergence is given by

$$\begin{aligned} \nabla_{\mathbf{v}_i} \cdot \mathbf{F}_i = & \frac{1}{v_i} \frac{\partial}{\partial \theta_i} \Gamma \Lambda \sin(\psi - \theta_i) \\ = & \frac{\Gamma}{v_i} \frac{\partial}{\partial \theta_i} \frac{1}{N} \sum_{j=0}^N \sin(\theta_j - \theta_i) \\ = & -\frac{\Gamma}{v_i} \frac{1}{N} \sum_{j \neq i} \cos(\theta_j - \theta_i) \\ = & \frac{\Gamma}{v_i} \left[ \frac{1}{N} - \Lambda \cos(\psi - \theta_i) \right]. \end{aligned} \quad (\text{B5})$$

Inserting the magnitude and the divergence of  $\mathbf{F}_i$  into (B3), we obtain Eq. (11).

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