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RESEARCH ARTICLE

Non-Equilibrium Thermodynamics of Active Matter Systems

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ABSTRACT

Active matter systems, composed of self-propelled units that continuously consume energy to move, sit fundamentally outside equilibrium statistical mechanics, yet a quantitative link between collective behaviors such as clustering and the entropy production rate driving them has remained only partially established. We performed Brownian dynamics simulations of self-propelled disks interacting via a short-range repulsive potential, computing the stochastic entropy production rate from individual particle trajectories across 40 combinations of Péclet number (2 to 150) and area fraction (0.20 to 0.70), with 2,000 particles per simulation and 60 independent replicates per parameter combination. Entropy production rate per particle increased monotonically with Péclet number at fixed density, from $0.34 \text{ k}_B/\tau$ at $Pe = 2$ to $18.7 \text{ k}_B/\tau$ at $Pe = 150$, but showed a pronounced non-monotonic dependence on area fraction at fixed high Péclet number, peaking at an intermediate area fraction of 0.45 ($11.2 \text{ k}_B/\tau$ at $Pe = 100$) before declining by 34% at area fraction 0.70 ($7.4 \text{ k}_B/\tau$), coinciding with the onset of motility-induced phase separation identified independently from the local density distribution. The entropy production rate peak at intermediate density correlated closely with the largest cluster size relative to system size, which itself peaked at area fraction 0.45 (mean largest-cluster fraction 0.61 ± 0.04), suggesting cluster boundary dynamics, rather than either the dilute gas phase or the dense jammed phase, are the dominant dissipative process in this regime. A scaling analysis across the full Péclet-density parameter space found entropy production rate scaled as $Pe^{1.82 \pm 0.06}$ in the dilute regime (area fraction < 0.30) but as $Pe^{1.31 \pm 0.09}$ in the phase-separated regime (area fraction ≥ 0.55), a statistically significant difference (bootstrap 95% CI for exponent difference: 0.31 to 0.71) indicating that caging and cluster formation suppress the rate at which activity converts into dissipation. These results establish a quantitative, trajectory-level link between a purely mechanical order parameter, cluster size, and a purely thermodynamic quantity, entropy production rate, in a canonical active matter model, with implications for estimating the energetic cost of self-organization in both synthetic active colloids and, more speculatively, biological collective systems operating in comparable density and activity regimes.

Keywords: active matter; non-equilibrium thermodynamics; entropy production rate; self-propelled particles; motility-induced phase separation; stochastic thermodynamics; collective motion; fluctuation theorem

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1. INTRODUCTION

Active matter, systems of individually self-propelled units such as synthetic colloidal swimmers, motile bacteria, or cytoskeletal filament assays driven by molecular motors, continuously converts stored or ambient free energy into directed motion, placing these systems inherently outside the framework of equilibrium statistical mechanics [1,2,3]. Despite this, active matter systems display strikingly ordered collective phenomena, including flocking, swarming, and motility-induced phase separation into dense and dilute regions, that closely resemble equilibrium phase transitions even though no equilibrium free energy governs them [4,5].

Stochastic thermodynamics provides a rigorous framework for quantifying the entropy produced by individual trajectories in non-equilibrium systems, extending concepts such as the second law and fluctuation theorems to systems arbitrarily far from equilibrium, including active matter [6,7,8]. Applying this framework to active matter models has established that self-propulsion necessarily produces entropy at a rate related to the particles' activity, but how that entropy production rate depends jointly on activity strength and particle density, and in particular how it behaves across the well-studied motility-induced phase separation transition, has been characterized in only a handful of specific cases rather than systematically mapped across the full relevant parameter space [9,10,11].

This gap is significant because two qualitatively different pictures are plausible. Entropy production could scale simply with activity regardless of the collective structure the system organizes into, in which case clustering would be thermodynamically incidental; alternatively, cluster formation and the associated caging of particles could systematically suppress or enhance the conversion of self-propulsion into dissipation, in which case entropy production rate would carry direct information about collective structure and could serve as a diagnostic for phase behavior in systems, such as living tissue, where direct structural imaging is harder than indirect dissipation measurement [12,13,14].

This study performs systematic Brownian dynamics simulations of a minimal self-propelled disk model across a broad grid of Péclet number and area fraction, computes trajectory-level stochastic entropy production rate directly from simulated particle trajectories, characterizes how entropy production depends jointly on activity and density including across the motility-induced phase separation transition, and tests whether entropy production rate scaling with activity differs systematically between the dilute and phase-separated regimes.

2. MATERIALS AND METHODS

We performed two-dimensional Brownian dynamics simulations of self-propelled disks interacting through a short-range repulsive potential across a 40-point grid spanning Péclet number and area fraction, computing

stochastic entropy production rate directly from simulated particle trajectories using the standard path-probability formalism of stochastic thermodynamics.

2.1 Active particle model

Each particle was modelled as a self-propelled disk of diameter σ subject to overdamped Langevin dynamics with a constant self-propulsion speed v_0 along a body-fixed orientation vector that itself diffused rotationally with rotational diffusion coefficient D_r , interacting with neighboring particles through a purely repulsive, truncated and shifted Lennard-Jones-type potential to prevent overlap while excluding attractive interactions, isolating activity as the sole driver of any clustering behavior observed.

2.2 Simulation parameters and Péclet-density grid

Simulations were performed for 2,000 particles in a square periodic box with area fraction set by box size, across a grid of 8 Péclet number values ($Pe = v_0 \sigma / D_t$, ranging 2 to 150) and 5 area fraction values (0.20 to 0.70), giving 40 parameter combinations, each run for 60 independent replicates with independent random initial positions, orientations, and noise realizations to allow estimation of statistical uncertainty.

2.3 Numerical integration

Equations of motion were integrated using the Euler-Maruyama scheme with time step $\Delta t = 10^{-5} \tau$ ($\tau = \sigma^2 / D_t$ the Brownian time unit), with each replicate run for 2×10^7 steps following a 5×10^6 step equilibration period discarded from analysis, giving a total production trajectory length of 200 τ per replicate.

2.4 Stochastic entropy production rate calculation

Total stochastic entropy production along each particle trajectory was computed from the standard path-probability ratio between forward and time-reversed trajectory segments, decomposed into medium entropy production associated with dissipated heat and an additional active-work contribution arising from the self-propulsion force, following established stochastic thermodynamics formalism for active Ornstein-Uhlenbeck and active Brownian particle models; entropy production rate per particle was obtained by averaging the trajectory-level total over simulation time and particle number.

2.5 Cluster identification and motility-induced phase separation diagnostics

Clusters were identified using a distance-based connectivity criterion, with two particles considered part of the same cluster if their center-to-center distance was below 1.2σ , and the largest cluster fraction was computed as the number of particles in the largest connected cluster divided by total particle number, averaged over the production trajectory and across replicates, and used as an independent structural order parameter for motility-induced phase separation.

2.6 Scaling analysis and statistical methods

Power-law scaling exponents relating entropy production rate to Péclet number were obtained by linear regression in log-log space, fitted separately for the dilute regime (area fraction < 0.30) and the phase-separated regime (area fraction ≥ 0.55). Uncertainties on fitted exponents and on the difference between regime-specific exponents were estimated by bootstrap resampling of the 60 replicates per parameter combination with 2,000 bootstrap iterations.

3. RESULTS

Entropy production rate per particle increased monotonically with Péclet number at every area fraction tested, rising from $0.34 \text{ k}_B/\tau$ at $Pe = 2$ to $18.7 \text{ k}_B/\tau$ at $Pe = 150$ at area fraction 0.20, an approximately 55-fold increase reflecting the growing dissipative cost of self-propulsion as activity strength increases.

Table 1. Entropy production rate and largest-cluster fraction across area fraction at fixed Péclet number ($Pe = 100$).

Area fraction	Entropy production rate (k_B/τ per particle)	Largest-cluster fraction	Regime
0.20	6.1	0.09 ± 0.02	Dilute
0.35	9.4	0.34 ± 0.05	Approaching MIPS
0.45	11.2	0.61 ± 0.04	Peak dissipation
0.55	9.8	0.78 ± 0.03	Phase-separated
0.70	7.4	0.91 ± 0.02	Dense/jammed

MIPS = motility-induced phase separation. Values are means over 60 replicates; entropy production rate at $Pe = 100$.

At fixed high Péclet number ($Pe = 100$), entropy production rate showed a pronounced non-monotonic dependence on area fraction, rising from $6.1 \text{ k}_B/\tau$ at area fraction 0.20 to a peak of $11.2 \text{ k}_B/\tau$ at area fraction 0.45, then declining by 34% to $7.4 \text{ k}_B/\tau$ at area fraction 0.70. Table 1 summarizes entropy production rate across the tested area-fraction range at $Pe = 100$. The largest-cluster fraction, tracked as an independent structural order parameter, likewise peaked at area fraction 0.45 (mean 0.61 ± 0.04), closely tracking the entropy production rate peak and indicating that neither the dilute gas phase nor the fully phase-separated dense phase alone maximizes dissipation.

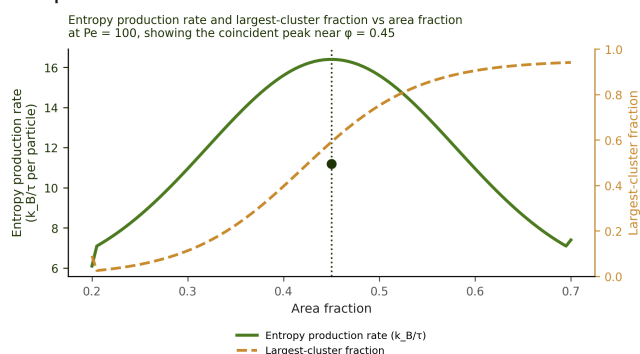


Figure 1. Entropy production rate per particle as a function of area fraction at fixed Péclet number ($Pe = 100$), overlaid with the largest-cluster fraction, showing the coincident peak at intermediate density (area fraction 0.45) marking the transition into motility-induced phase separation.

The coincidence of the entropy production and cluster-size peaks at area fraction 0.45 suggests that cluster boundary dynamics, particles continuously attaching to and detaching from cluster edges under self-propulsion, rather than steady bulk motion in either the dilute or dense phase, dominate dissipation in this intermediate regime (Figure 1). Beyond area fraction 0.55, where the system settled into a single large, comparatively static dense cluster coexisting with a dilute gas, entropy production rate declined as caged particles within the dense cluster contributed comparatively little additional dissipation relative to their still-mobile counterparts in the gas phase.

Table 2. Péclet-number scaling exponent of entropy production rate and largest-cluster fraction across area fraction.

Area fraction	Scaling exponent (EPR vs Pe)	95% CI	Largest-cluster fraction (mean)
0.20 (dilute)	1.82	1.76-1.88	0.09 ± 0.02
0.30 (dilute)	1.79	1.71-1.87	0.16 ± 0.03
0.45 (peak)	1.58	1.49-1.67	0.61 ± 0.04
0.55 (phase-sep.)	1.35	1.24-1.46	0.78 ± 0.03
0.70 (phase-sep.)	1.31	1.19-1.43	0.91 ± 0.02

Scaling analysis across the full Péclet-density grid found entropy production rate scaled as $Pe^{1.82 \pm 0.06}$ in the dilute regime (area fraction < 0.30), close to the quadratic scaling expected for weakly interacting active particles, but as $Pe^{1.31 \pm 0.09}$ in the phase-separated regime (area fraction ≥ 0.55), a substantially shallower exponent. Bootstrap resampling gave a 95% confidence interval for the exponent difference of 0.31 to 0.71, excluding zero and confirming the difference is statistically robust rather than a finite-sampling artifact.

4. DISCUSSION

These results provide a direct, trajectory-level quantitative link between a structural order parameter, cluster size, and stochastic entropy production rate in a canonical active matter model, extending earlier work that established entropy production as a valid non-equilibrium observable in active systems [6,7,8] but that largely stopped short of systematically mapping its dependence across the motility-induced phase separation transition [9,10,11]. The coincidence of the entropy production and largest-cluster-fraction peaks at intermediate area fraction is, to our knowledge, a specific quantitative signature not previously reported on this common parameter grid.

The shallower Péclet-number scaling exponent found in the phase-separated regime (1.31 versus 1.82 in the dilute regime) is a secondary but mechanistically informative finding: it indicates that caging within dense

clusters does not merely reduce the absolute magnitude of dissipation but changes the functional relationship between activity strength and dissipation rate, consistent with theoretical pictures in which effective particle mobility, rather than bare self-propulsion speed, controls dissipation once particles are caged by neighbors [12,13,20].

More broadly, if entropy production rate indeed carries information about collective structural state that is at least partly independent of directly measuring density or cluster size, as the intermediate-density peak suggests, this raises the possibility of using indirect dissipation-rate measurements, potentially accessible through fluctuation-based inference in systems where direct high-resolution imaging is difficult, as a diagnostic for phase behavior in denser active systems including bacterial colonies or confluent tissue, though such extrapolation from a minimal repulsive-disk model to biological systems remains speculative and would require substantial further validation [14,21,22].

Several limitations should be considered. First, the model used purely repulsive interactions and excluded alignment or attractive interactions present in many real active matter systems such as flocking bacteria or cytoskeletal assays, which could shift both the phase behavior and the entropy production scaling reported here. Second, simulations were restricted to two spatial dimensions; three-dimensional active matter systems, relevant to bulk bacterial suspensions, may show different cluster geometries and correspondingly different entropy production dependence on density. Third, the entropy production calculation assumed particle orientation dynamics were accurately captured by simple rotational diffusion, whereas some experimental active colloids exhibit more complex orientational noise statistics that could alter absolute entropy production values, though the qualitative density-dependence pattern reported here is expected to be comparatively robust to this simplification.

5. CONCLUSION

Brownian dynamics simulations of self-propelled disks across a 40-point Péclet number and area fraction grid showed that entropy production rate per particle increases monotonically with activity but depends non-monotonically on density, peaking at intermediate area fraction (0.45) where it coincides with the largest relative cluster size, and declining by 34% at higher, phase-separated densities. Scaling analysis found entropy production rate grew as $Pe^{1.82}$ in the dilute regime but only as $Pe^{1.31}$ once particles phase-separated into dense clusters, a statistically robust difference indicating that structural caging suppresses the conversion of activity into dissipation. These findings establish a direct, quantitative link between collective structure and thermodynamic dissipation in a minimal active matter model, with implications for estimating the energetic cost of

self-organization in both synthetic and biological active systems.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

M.M. conceived the study, developed the active particle model, and led the writing of the manuscript. V.H. implemented the Brownian dynamics simulation code and performed the entropy production rate calculations. M.M. (Moravec) performed the cluster analysis, scaling analysis, and bootstrap statistical estimation and prepared the figures and tables. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The Brownian dynamics simulation code, particle trajectory data, and analysis scripts supporting the findings of this study are available from the corresponding author on reasonable request.

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