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Configurational entropy and effective temperature in systems of active Brownian particles†

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We propose a method to determine the effective density of states and configurational entropy in systems of active Brownian particles by measuring the probability distribution function of potential energy at varying temperatures. Assuming that the entropy is a continuous and monotonically increasing function of energy, we provide support that two-dimensional systems of purely repulsive active Brownian spheres can be mapped onto an equilibrium system with a Boltzmann-like distribution and an effective temperature. We find that the effective temperature depends even for a large number of particles on system size, suggesting that active systems are non-extensive. In addition, the effective Helmholtz free energy can be derived from the configurational entropy. We verify our results regarding the configurational entropy by using thermodynamic integration of the effective Helmholtz free energy with respect to temperature.

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Introduction

Very recently, there has been a huge shift in interest from passive to active colloidal systems.^{1–10} In contrast to passive colloidal particles that only exhibit Brownian motion due to thermal fluctuations, active self-propelled colloids are driven by an intricate interplay between random fluctuations and active swimming. While passive Brownian particles are in thermodynamic equilibrium with the solvent, thereby satisfying the fluctuation-dissipation theorem, active particles are driven far from equilibrium as they incessantly convert energy into active motion that gets dissipated through viscous damping. These active systems display a number of compelling features not typical for equilibrium systems such as dynamical phase transitions^{11–15} or anomalous diffusion.¹⁶ Yet, they also show behavior very similar to equilibrium systems, *e.g.* out-of-equilibrium analogs of crystals, liquids, and gases, including phase coexistence, nucleation, and spinodal composition,^{4,6,17–21} which motivated many researchers to describe these systems using the framework of equilibrium statistical mechanics.^{22–24} However, recent attempts show that even basic thermodynamic properties such as non-equilibrium equivalents of temperature and pressure depend sensitively on the precise definitions at hand, *e.g.*, the mechanical pressure (force per unit area exerted on a wall), thermodynamic pressure (derivative of the free energy with respect to volume), or hydrodynamic pressure (trace of the

bulk stress tensor) do not necessarily correspond to each other in out-of-equilibrium systems,^{25–29} the same is true for various definitions of temperature, *e.g.* using diffusion,¹⁰ fluctuation-dissipation theorem,^{30,31} and others.^{32–34} So far there is no consensus on how to define the pressure and temperature in active matter and there is yet no clear statistical mechanics framework for active systems.

In this article, we propose a method to determine an effective non-equilibrium equivalent of the density of states, $\Omega_{\text{NE}}(U)$, hence the effective configurational entropy, $S_{\text{NE}}(U)$, in systems of active Brownian spheres by measuring the probability distribution function $P_{\text{NE}}(U)$ of potential energy U for varying reduced temperatures T' of the particle system. By assuming that the entropy is a continuous and monotonically increasing function of U , we provide support that active systems can be mapped onto an equilibrium system with a many-particle distribution function that resembles the Boltzmann distribution, but with an effective temperature instead. In addition, the corresponding effective Helmholtz free energy can be derived from the configurational entropy, which may allow us to determine the thermodynamics and phase behavior of active Brownian particles. Moreover, we verify our results of the configurational entropy using a different route based on thermodynamic integration of the effective free energy with respect to temperature.

Model

We consider a two-dimensional system of N active Brownian spheres interacting with a purely repulsive Weeks–Chandler–Andersen

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(WCA) potential in thermodynamic equilibrium with a heat bath at temperature T . The WCA interaction potential $\mathcal{U}_{\text{WCA}}(r)$ reads

$$\mathcal{U}_{\text{WCA}}(r_{ij}) = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] + \varepsilon & \text{if } r_{ij} < 2^{1/6}\sigma \\ 0 & \text{if } r_{ij} \geq 2^{1/6}\sigma \end{cases} \quad (1)$$

where r_{ij} is the distance between particles i and j , ε is the interaction strength and σ is our unit of length. The motion of particle i at position \mathbf{r}_i and velocity $\dot{\mathbf{r}}_i$ is described by the overdamped Langevin equation

$$\dot{\mathbf{r}}_i(t) = \frac{D_t}{k_B T} [-\nabla_i U(t) + f\mathbf{e}_i(t)] + \sqrt{2D_t} \boldsymbol{\Gamma}_i(t), \quad (2)$$

where the potential energy $U = \sum_{i < j} \mathcal{U}_{\text{WCA}}(r_{ij})$ is the sum of WCA

interactions between all active spheres and $D_t = k_B T / \gamma$ is the translational diffusion coefficient with γ being the translational friction coefficient. A stochastic force with zero mean, $\boldsymbol{\Gamma}(t)$, describes the collisions with the solvent molecules, and satisfies $\langle \Gamma_{\alpha,i}(t) \Gamma_{\beta,j}(t') \rangle = \delta_{\alpha\beta} \delta_{ij} \delta(t - t')$ with $\alpha, \beta = x, y, z$. In addition, the self-propulsion of particle i is described by a constant force f in the direction $\mathbf{e}_i(t)$ at time t . The orientation $\mathbf{e}_i(t)$ of particle i undergoes free Brownian rotation according to $\dot{\mathbf{e}}_i(t) = \sqrt{2D_r} (\mathbf{e}_i(t) \times \boldsymbol{\Gamma}_i^r(t))$, where D_r denotes the rotational diffusion coefficient and $\boldsymbol{\Gamma}_i^r(t)$ is a Gaussian white-noise random vector, which satisfies $\langle \Gamma_{\alpha,i}^r(t) \rangle = 0$ and $\langle \Gamma_{\alpha,i}^r(t) \Gamma_{\beta,j}^r(t') \rangle = \delta_{\alpha\beta} \delta_{ij} \delta(t - t')$. In addition, we define the temperature of our system of active Brownian spheres by a dimensionless temperature $T' = k_B T / \varepsilon$, which we vary by changing the interaction strength ε in the WCA potential (1). Please note that changing the temperature T of the heat bath changes not only the temperature of the particle system through $T' = k_B T / \varepsilon$, but also the magnitude of the Brownian noise and thus the system dynamics. We therefore kept the temperature T of the Brownian bath constant as well as the translational diffusion coefficient D_t and rotational diffusion coefficient D_r , and changed the temperature of the particle system only by changing ε . Exemplarily, we show typical configurations of the active system with 512 particles in Fig. 1 for density $\rho\sigma^2 = 0.5$, temperature $T' = 1$, and varying self-propulsion forces $f\sigma/k_B T = 0, 6.35, 10.08$, and 25.4. We clearly observe that the system becomes more heterogeneous upon increasing the activity.

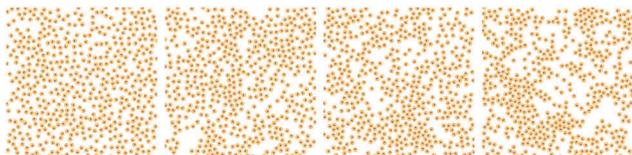


Fig. 1 Typical configurations of a system of $N = 512$ active Brownian spheres at a number density $\rho\sigma^2 = 0.5$, reduced temperature $T' = k_B T / \varepsilon = 1$, and varying self-propulsion forces $f\sigma/k_B T = 0, 6.35, 10.08$, and 25.4 from left to right.

Results

Configurational entropy in an equilibrium system

In order to investigate the configurational entropy $S(U)$ we use the direct histogram method³⁵ and the thermodynamic integration technique.³⁶ Both methods are standard techniques used in simulations of equilibrium systems. Below, we describe them first for equilibrium systems, and explain then how we extend them to active systems. In ref. 35, a method was devised for calculating the density of states $\Omega(U)$ and the configurational entropy function $S(U)$ directly from simulation data. In this method, $\Omega(U)$ and $S(U)$ are determined from the probability distribution function of energy $P(U)$ with U being the potential energy of the system due to the particle interactions. $P(U)$ is measured from simulations in a canonical ensemble, *i.e.*, the number of particles N , the volume V , and the temperature T are fixed. In the canonical ensemble, $P(U)$ reads

$$P(U|N, V, T) = \frac{\Omega(U, V, N) e^{-U/k_B T}}{Q(N, V, T)}, \quad (3)$$

where $Q = \int d\mathbf{r}^N \exp[-U/k_B T]$ denotes the configurational part of the partition function. The configurational entropy $S(U)$ can be obtained directly from

$$S(U, V, N) = k_B \ln \Omega(U, V, N). \quad (4)$$

From eqn (4), it is straightforward to obtain the difference in entropy $\Delta S_{IJ} = S(U_I) - S(U_J)$ between states I and J with energies U_I and U_J , respectively

$$\Delta S_{IJ}/k_B = \ln \frac{P(U_I|N, V, T)}{P(U_J|N, V, T)} + (U_I - U_J)/k_B T. \quad (5)$$

We note that ΔS_{IJ} is independent of the configurational partition function $Q(N, V, T)$. Eqn (5) is the key equation here, which we employ to probe the system statistics. In order to determine the entropy function $S(U)$, we measure $P(U)$ for varying reduced temperatures $T' = k_B T / \varepsilon$ of the particle system. The temperatures are chosen such that the energy distributions overlap. The entropy function is then recovered by solving consecutively eqn (5) for energy states I and $J = I + 1$ for all I . To this end, we perform Brownian dynamics simulations of $N = 512$ passive WCA particles at a number density $\rho\sigma^2 = 0.7$. The self-propulsion force $f\sigma/k_B T = 0$ and the simulations correspond to an equilibrium system. We measure $P(U)$ for varying T' , and present the results in Fig. 2a. We observe that the maximum of $P(U)$ shifts to higher energies upon increasing T' as expected. In addition, the distributions become broader with T' . In Fig. 2b we show the average potential energy $\langle U/\varepsilon \rangle$ as a function of reduced inverse temperature $1/T'$ and we fit the data with a spline as denoted by the blue line. Using eqn (5), we determine the difference in configurational entropy $\Delta S_{IJ}/k_B$ between energy states U_I and U_J as a function of $U = (U_I + U_J)/2$ with $J = I + 1$ and for all I . We fix the energy difference $\Delta U_{IJ} = U_I - U_J = 0.71\varepsilon$, and plot the results in Fig. 2c. We clearly find that the entropy differences ΔS_{IJ} as obtained from Brownian dynamics simulations at varying T' nicely overlap. Finally, we obtain the configurational entropy $S(U)$ as a

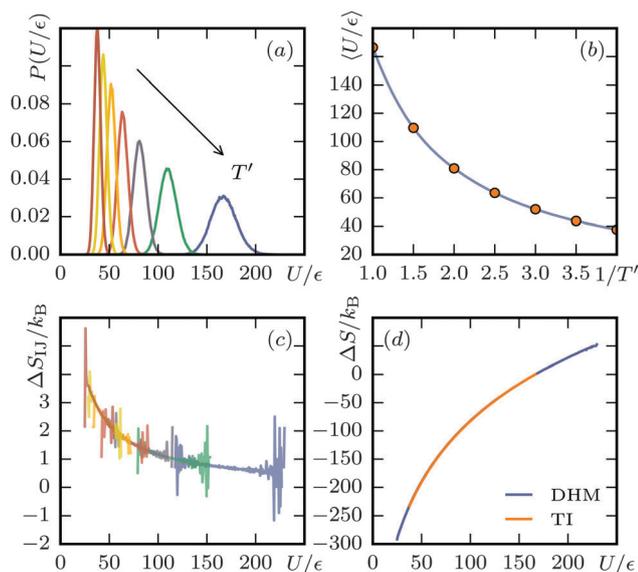


Fig. 2 (a) Probability distribution function $P(U/\epsilon)$ of potential energy U for varying reduced temperatures $T' = k_B T/\epsilon = 0.25, 0.286, 0.33, 0.4, 0.5, 0.67$, and 1.0 in the direction denoted by the arrow as obtained from Brownian dynamics simulations of a system of $N = 512$ passive WCA particles and number density $\rho\sigma^2 = 0.7$. (b) The averaged potential energy $\langle U/\epsilon \rangle$ as a function of $1/T'$. The orange dots correspond to measured averages. The blue line is a spline fit, which is used for the thermodynamic integration. (c) The entropy difference $\Delta S_{ij}/k_B$ between energy states U_i and U_j as a function of $U = (U_i + U_j)/2$ with $J = I + 1$. The energy difference $\Delta U_{ij}/\epsilon = 0.71$ is kept fixed for all I . (d) The entropy $\Delta S(U)/k_B = (S(U) - S(U^*))/k_B$ as a function of energy U with $U^* = 162.38\epsilon$ as obtained from the direct histogram method (blue line) and the thermodynamic integration method (red).

function of energy U by summing up ΔS_{ij} sequentially for increasing I as plotted in Fig. 2d. As expected, we observe that $S(U)$ is a continuous and monotonically increasing function of U . We verify our results of the entropy by using thermodynamic integration of the Helmholtz free energy $F = U - TS$ with respect to the inverse temperature

$$\frac{F(N, V, T'_2)}{T'_2} - \frac{F(N, V, T'_1)}{T'_1} = \int_{1/T'_1}^{1/T'_2} \langle U \rangle d(1/T'). \quad (6)$$

Using the spline fit $U(1/T')$ as shown in Fig. 2b in eqn (6), it is straightforward to obtain the difference in entropy, which we plot in Fig. 2d for comparison with the direct histogram method. We find a perfect agreement between the two methods.

Non-equilibrium equivalent of configurational entropy

Now we turn our attention to active systems. There are different approaches that can be chosen to describe steady states in out-of-equilibrium systems. One approach is to construct an effective Hamiltonian that generates a Liouville distribution in an equilibrium system that closely resembles that of the non-equilibrium system of interest, *i.e.*, the same (or nearly the same) configurational phase space distribution function is sampled by both dynamics and it thus captures in an equilibrium system the static properties of the out-of-equilibrium system. The advantage

of such an approach is that the framework of statistical mechanics can readily be employed, see *e.g.*, ref. 22–24 and 37. In this article, we investigate the statistics of the out-of-equilibrium system of active Brownian disks, and suggest that the steady state of an active system can be mapped onto an equilibrium system with a Boltzmann-like distribution with the potential energy given by the bare particle interactions instead of the unknown effective interactions, but with an effective temperature.

To this end, we assume that the probability $P_{\text{NE}}(U)$ to find our non-equilibrium (NE) system in a steady-state with potential energy U can be written in a similar way as in eqn (3), where the Boltzmann–Gibbs measure is replaced by an unknown measure that is determined by the dynamics. We note here that such an alternative can be formulated, at least formally, for deterministic systems, where the dynamical measure is defined by the phase space trajectories.³⁸ Unfortunately, we are not aware of such an expression for stochastic systems like the active Brownian spheres. In order to proceed we consider a probability weight $g(U)$ by analogy with equilibrium systems, which depends only on the potential energy U of the steady states that are sampled by the dynamics of the system.

$$P_{\text{NE}}(U|N, V, T', D_t, D_r, f) = \frac{\Omega_{\text{NE}}(U, V, N)g(U)}{Q_{\text{NE}}(N, V, T', D_t, D_r, f)}, \quad (7)$$

where $P_{\text{NE}}(U)$ is a probability distribution of the potential energy U generated by the out-of-equilibrium dynamics. This probability distribution is, however, dependent on all parameters that determine the dynamics of the particle system *i.e.* N, V, T', D_t, D_r and f . Furthermore, $Q_{\text{NE}} = \int d\mathbf{r}^N g(U)$ denotes the non-equilibrium configurational part of the partition function and $\Omega_{\text{NE}}(U, V, N)$ the effective non-equilibrium density of states of the non-equilibrium system. There are a few remarks that we wish to make. We first note that $P_{\text{NE}}(U)$ denotes the probability of finding a configuration in a steady state with potential energy U . Since U depends only on the positions of particles in the system and not on the instantaneous momenta of the particles, we have basically integrated out the momenta of the particles. Note, however, that the kinetic contributions to U and S are trivial for equilibrium systems on which we map our active system, but this might not be true for the original out-of-equilibrium system. Secondly, we assume that the integral $Q_{\text{NE}} = \int d\mathbf{r}^N g(U)$ holds and that the system is ergodic. By requiring this we neglect the system's dissipation and its consequences. Within this interpretation, our approach can be considered as a mapping of the steady state of an out-of-equilibrium system onto an effective equilibrium one.

We now assume that $g(U)$ is still exponential in U , but with an effective temperature T_{eff}

$$g(U) = \exp[-U/(k_B T_{\text{eff}})] \quad (8)$$

with $U = \sum_{i < j} U_{\text{WCA}}(r_{ij})$. We thus assume that the many-particle configurational probability distribution depends only on the potential energy due to the bare particle interactions, which is

valid in the limit of weakly persistent motion, *i.e.*, the persistence time $\tau = D_t/(2D_r\sigma^2) \rightarrow 0$.^{22–24}

The effective temperature is thus a consequence of the non-equilibrium dynamics and depends on all system parameters N , V , T' , D_t , D_r and f . In the limit of $f\sigma/k_B T \rightarrow 0$, our active system reduces to an equilibrium system with the Boltzmann statistics and with $T_{\text{eff}} \rightarrow T'$. In the absence of interactions or in the limit of weakly persistent motion the effective temperature can be expressed as $T_{\text{eff}} = T'(1 + v_0^2/2D_r D_t)$, also called the swim temperature^{22–24} with $v_0 = fD_t/k_B T$. Hence, the effective temperature should be in the range $1 \leq T_{\text{eff}}/T' \leq 1 + v_0^2/2D_r D_t$. We wish to note here that many extensions of a more generalized statistics for dynamical systems reduce to a Boltzmann-like weight with an effective temperature provided the fluctuations are sufficiently small.³⁹ Moreover, recent work on sedimentation or centrifugation of active colloidal suspensions supports the concept of an effective temperature in active systems.^{1,40–42} In order to investigate if the energy probability distribution function (7) can be described by an alternative measure, in our case represented by the probability weight (8) with an effective temperature T_{eff} , we measure $P_{\text{NE}}(U|N, V, T)$ in Brownian dynamics simulations of $N = 512$ active particles with a self-propulsion force $f\sigma/k_B T = 10$, number density $\rho\sigma^2 = 0.7$, and rotational diffusion coefficient $D_r = D_t/\sigma^2$. We plot $P_{\text{NE}}(U)$ for

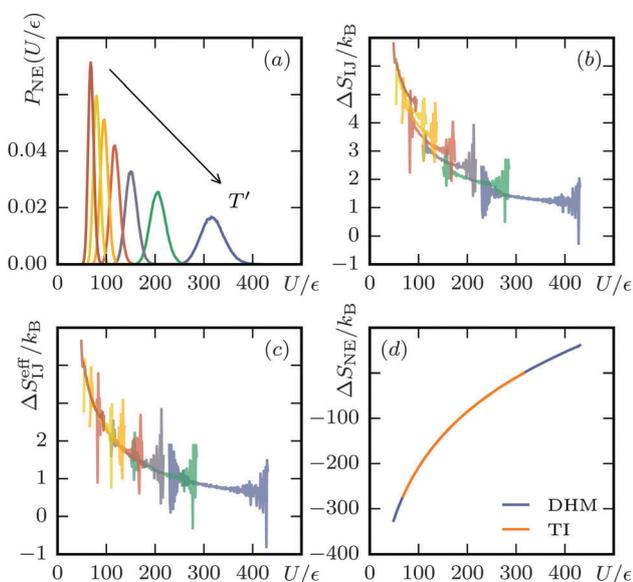


Fig. 3 (a) Probability distribution functions $P_{\text{NE}}(U/\epsilon)$ for a system of $N = 512$ WCA particles with a self-propulsion force $f\sigma/k_B T = 10$, number density $\rho\sigma^2 = 0.7$, and rotational diffusion coefficient $D_r = D_t/\sigma^2$ for varying reduced temperatures $T' = k_B T/\epsilon = 0.25, 0.286, 0.33, 0.4, 0.5, 0.67$, and 1.0 in the direction denoted by the arrow. (b) The entropy difference $\Delta S_{ij}/k_B$ between energy states U_i and U_j as a function of $U = (U_i + U_j)/2$ with $J = I + 1$ as obtained from eqn (5) The entropy differences are not overlapping for varying T' . (c) $\Delta S_{ij}^{\text{eff}}/k_B$ as a function of $U = (U_i + U_j)/2$, but assuming an effective temperature $T_{\text{eff}}/T' = 1.67$. The curves are overlapping well within our statistical accuracy. The energy difference $\Delta U_{ij} = 1.33\epsilon$ is kept fixed for all I . (d) The relative effective entropy $\Delta S_{\text{NE}}(U)/k_B = (S_{\text{NE}}(U) - S_{\text{NE}}(U^*))/k_B$ as a function of energy U with $U^* = 315.35\epsilon$ as obtained from the direct histogram method (blue line) and the thermodynamic integration method (red line).

varying T' in Fig. 3a, which are shifted to higher energy values with respect to a passive system due to the activity of the particles. Assuming an ordinary Boltzmann distribution and employing naively the direct histogram method as described by eqn (5) for an equilibrium system, we clearly observe in Fig. 3b that the entropy differences ΔS_{ij} for fixed $\Delta U_{ij}/\epsilon = 1.33$ are not overlapping for varying T' as the steady-state of the out-of-equilibrium system is not described by an ordinary Boltzmann statistics with potential energy U . If we assume that ΔS_{ij} should be a continuous function of U and we replace T' with an effective temperature $T_{\text{eff}}/T' = a$, we recover the perfect overlap of $\Delta S_{ij}^{\text{eff}}$ as shown in Fig. 3c with just a single fit parameter $a = 1.67$ for all seven different temperatures T' that we considered. We thus find that $T_{\text{eff}} > T'$ due to the self-propulsion, but $T_{\text{eff}}/T' < (1 + v_0^2/2D_r D_t) = 51$ as a result of the particle interactions. Summing up $\Delta S_{ij}^{\text{eff}}$ sequentially, we obtained $S_{\text{NE}}(U)$ as shown in Fig. 3d. We again compare our results with thermodynamic integration, where we use the effective temperature as obtained from the direct histogram method in eqn (6). We find a perfect match between the two methods, thereby providing support for the Boltzmann-like probability weight (8) and an effective temperature. We thus use the effective temperature T_{eff} not only as a fit parameter, but it also has a thermodynamic meaning since $1/T_{\text{eff}} = \partial S_{\text{NE}}/\partial U$ by construction.

In addition, we investigate the effect of system size on the resulting T_{eff} using this approach. In Fig. 4a, we plot T_{eff} for a system of WCA particles with a self-propulsion force $f\sigma/k_B T = 10$, number density $\rho\sigma^2 = 0.5$ and rotational diffusion coefficient $D_r = D_t/\sigma^2$ as a function of system size N . We observe that T_{eff} is strongly dependent on N even for large system sizes up to 8192 particles and keeps on increasing with N . Fig. 4a suggests that these active systems are non-extensive, which would be in agreement with previous studies on granular matter, where extensivity has been investigated using similar approaches.^{43–45} However, as it becomes more difficult to measure the effective temperature for larger system sizes, it would be interesting for future work to employ more precise methodologies to calculate the system size dependence of the effective temperature.

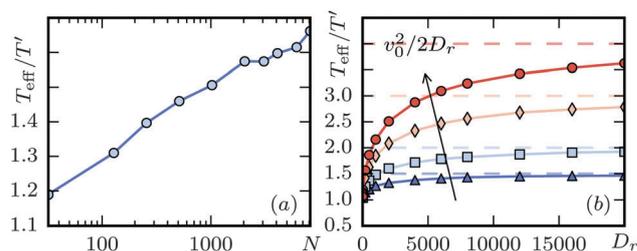


Fig. 4 (a) The effective temperature T_{eff}/T' as a function of N on a logarithmic scale for WCA particles with self-propulsion $f\sigma/k_B T = 10$, $D_r = D_t/\sigma^2$ and number density $\rho\sigma^2 = 0.5$. (b) T_{eff}/T' as a function of $D_r\sigma^2/D_t$ for WCA particles with number density $\rho\sigma^2 = 0.5$, $N = 1024$, and varying $v_0^2/2D_r D_t = 0.5, 1, 2$, and 3 from bottom to top as denoted by the arrow. For large $D_r\sigma^2/D_t$ we recover the weakly persistent motion regime with the effective temperature $T_{\text{eff}}/T' = 1 + v_0^2/2D_r D_t$ as denoted by the horizontal dashed lines.

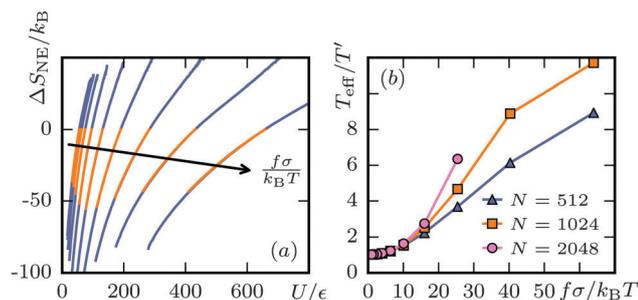


Fig. 5 (a) The relative effective entropy $\Delta S_{\text{NE}}/k_{\text{B}} \equiv S_{\text{NE}}(U)/k_{\text{B}} - S_{\text{NE}}(U^*)/k_{\text{B}}$ as a function of energy U/ϵ as obtained from the direct histogram method (blue line) and the thermodynamic integration method (orange line) for a system of $N = 512$ active Brownian spheres with varying self-propulsion forces $f\sigma/k_{\text{B}}T = 1.00, 1.59, 2.52, 4.00, 6.35, 10.08, 16.00, 25.40, 40.32,$ and 64.00 as denoted by the arrow, rotational diffusion $D_r = D_t/\sigma^2$ and number density $\rho\sigma^2 = 0.5$. (b) The effective temperature T_{eff}/T' as a function of self-propulsion force $f\sigma/k_{\text{B}}T$ as obtained from the direct histogram method for varying number of particles $N = 512, 1024,$ and 2048 as labeled for a system of $N = 512$ active Brownian spheres at number density $\rho\sigma^2 = 0.5$ and rotational diffusion coefficient $D_r = D_t/\sigma^2$.

Our results thus show that care has to be taken with finite-size effects in active systems.

Additionally, we determine the effective temperature as a function of rotational diffusion coefficient D_r in order to study the limit of weakly persistent motion for which $T_{\text{eff}}/T' \rightarrow 1 + v_0^2/2D_rD_t$.^{22–24,46} To this end we fix $v_0^2/2D_rD_t = 0.5, 1, 2, 3$ while changing the rotational diffusion D_r . Fig. 4b shows T_{eff}/T' as a function of D_r for a system of WCA particles with a self-propulsion force $f\sigma/k_{\text{B}}T = 10$, number density $\rho\sigma^2 = 0.5$, and $N = 1024$. We clearly observe that T_{eff}/T' increases from ~ 1 at low rotational diffusion D_r to $1 + v_0^2/2D_rD_t$ as denoted by the dashed horizontal lines in the limit of high D_r .

Additionally, we studied the effect of the self-propulsion force $f\sigma/k_{\text{B}}T$ on T_{eff} as shown in Fig. 5 for a system of $N = 512$ particles with $\rho\sigma^2 = 0.5$ and $D_r = D_t/\sigma^2$. As expected T_{eff} increases with activity, which can also be seen in Fig. 5a as the slope of

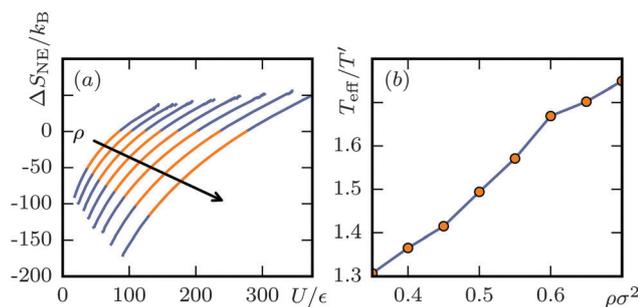


Fig. 6 (a) The relative effective entropy $\Delta S_{\text{NE}}/k_{\text{B}} \equiv S_{\text{NE}}(U)/k_{\text{B}} - S_{\text{NE}}(U^*)/k_{\text{B}}$ as a function of energy U/ϵ as obtained from the direct histogram method (blue line) and the thermodynamic integration method (orange line) for a system of $N = 450$ active Brownian spheres with self-propulsion forces $f\sigma/k_{\text{B}}T = 10$ and varying number densities $\rho\sigma^2 = 0.35, 0.4, 0.45, 0.5, 0.55, 0.6, 0.65,$ and 0.7 as denoted by the arrow and rotational diffusion $D_r = D_t/\sigma^2$. (b) The effective temperature T_{eff}/T' as a function of $\rho\sigma^2$ as obtained from the direct histogram method.

$\partial S_{\text{NE}}/\partial U = 1/T_{\text{eff}}$ decreases with self-propulsion. It is worth mentioning that for low activity $f\sigma/k_{\text{B}}T < 10$, we clearly see that the effective temperature becomes intensive, which can be appreciated by the data collapse in Fig. 5b for various system sizes. For $f\sigma/k_{\text{B}}T > 10$, T_{eff} becomes strongly dependent on system size as shown in Fig. 5b. However, in this case the system becomes inhomogeneous and is close to a motility-induced phase separation.

Finally, we also study T_{eff}/T' as a function of $\rho\sigma^2$ for a system of $N = 450$ particles. Surprisingly, we find that the configurational probability distribution is well described by a Boltzmann-like distribution as illustrated in Fig. 6a, but the effective temperature T_{eff}/T' increases with density $\rho\sigma^2$, see Fig. 6b. This seems to be at odds with our naive interpretation that the mobility decreases, and hence the “kinetic” effective temperature, with increasing density due to the interactions between the particles,²⁴ but we note here that the potential energy also increases with density as the particles interact more strongly at higher densities yielding a higher “thermodynamic” effective temperature.

Conclusions

In conclusion, we propose a method to determine the configurational entropy and probe the statistics of the many-particle configurational distribution functions in simulations of out-of-equilibrium systems. Assuming that the entropy is a continuous function of the potential energy, we lend support that systems of repulsive active Brownian spheres can be mapped onto an equilibrium system described by a Boltzmann-like distribution with the potential energy given by the bare particle interactions, and an effective temperature determined by an effective mobility that depends on the activity and interactions between the particles. We wish to remark here that in ref. 22–24 and 37 a different approach was adopted, in which the temperature is kept constant in the mapping or fixed to the swim temperature, but the effect of the dynamics due to self-propulsion, rotational diffusion, and particle interactions is casted into an effective Hamiltonian. It is tempting to speculate that the two descriptions are different sides of the same coin in which the combination $U_{\text{eff}}/k_{\text{B}}T_{\text{eff}}$ is key: one can either map the active system onto an effective equilibrium system with effective interactions and a fixed temperature, or one can keep the bare interactions but use instead an effective temperature. This demonstrates that the temperature is not uniquely defined for active systems. It would be interesting to measure the probability distribution functions of the potential energy of active systems using the effective Hamiltonian as presented in ref. 22–24 or to determine the effective interactions from structural input obtained from simulations of active systems,³⁷ which will be left for future studies.

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