Additivity and density fluctuations in Vicsek-like models of self-propelled particles

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We study coarse-grained density fluctuations in paradigmatic Vicsek-like models of self-propelled particles with alignment interactions and random self-propulsion velocities. By numerically integrating a fluctuation-response relation - a direct consequence of an additivity property, we compute logarithm of the large-deviation probabilities of coarse-grained subsystem density, called the large deviation functions, while the system is in a disordered fluid phase with vanishing macroscopic velocity. The large-deviation functions, computed within additivity, agree remarkably well with that obtained from direct microscopic simulations of the models. Our results provide an evidence of the existence of an equilibrium-like chemical potential, which governs density fluctuations in the Vicsek-like models.

I. INTRODUCTION

Large-scale behaviors of self-propelled particles, such as bacterial colony, fish schools, flocks of birds, swarm of insects or an assembly of photo-activated Janus particles - collectively called active matters, have drawn much attention in the past [1,2]. Self-propelled particles usually propel themselves by converting their internal chemical energy to mechanical one, which is then dissipated in the surrounding medium. They can be point-like, rod-like or spherical in shape, and polar or apolar in nature. Due to the mechanism of self-propulsion, such a system remains inherently out of equilibrium and could eventually reach a nonequilibrium steady state, which, in an intriguing manner, is far from being fully understood. Not surprisingly, a suitable statistical mechanics framework for active matters, though highly desirable, remains elusive. In this scenario, we show that a class of self-propelled particles with Vicsek-like interactions has a simple thermodynamic characterization in terms of an equilibrium-like additivity property.

According to standard formulation of statistical mechanics for an equilibrium system [27], where detailed balance is obeyed and consequently currents vanish, probability weights of microscopic configurations are provided by the Boltzmann-Gibbs distributions, irrespective of the details of microscopic dynamics of the system. In other words, in equilibrium, probabilities of microscopic configurations are a priori known and, therefore, can be readily used to determine macroscopic properties of the system. However, there is no such unified principle for systems having a nonequilibrium steady state - arguably the closest counterpart to equilibrium. Indeed, due to the violation of detailed balance, the probability weights of microscopic configurations in a nonequilibrium steady state in general cannot be described by the Boltzmann-Gibbs distribution. Moreover, they are usually a priori not known and have to be obtained from the microscopic dynamics of the systems. The difficulties begin precisely at this stage: In the absence of the knowledge of the steady-state probability weights, it is in principle not possible in nonequilibrium to relate the macroscopic properties of a system to the microscopic ones. Quite encouragingly though, an equilibrium-like approach to construct a thermodynamic framework has recently emerged for characterizing a broad class of nonequilibrium systems, that do not obey detailed balance and are not described by the Boltzmann-Gibbs distributions [28-31].

Thermodynamic property of additivity implies that, on a large scale, a system can be divided into many subsystems, which are statistically almost independent, except certain constraints due to conservation laws, e.g., conservation of mass or particle number, etc. Additivity property is well established in equilibrium systems with intensive thermodynamic variable, such as temperature [16], chemical potential [15,17] or pressure [18]. In a slightly different direction, there have been several studies to understand steady-state properties of self-propelled particles by using the methods of stochastic thermodynamics [19], where one attempts to quantify violation of time-reversibility by defining an entropy production [20-23]. Though such an approach is quite promising, the definition of entropy production may not be unique due to the coarse-graining involved in the microscopic dynamics of such systems [24-26].

Indeed, one major goal of constructing a steady-state thermodynamics is to understand fluctuations in systems having a nonequilibrium steady state. However, the exact nature of fluctuations in active matter systems, especially that of a conserved quantity, such as particle number, is far from being fully understood. Not surprisingly, a suitable statistical mechanics framework for active matters, though highly desirable, remains elusive. In this scenario, we show that a class of self-propelled particles with Vicsek-like interactions has a simple thermodynamic characterization in terms of an equilibrium-like additivity property.
port processes, having nonzero spatial correlations, can possess an additivity property in their respective steady states. As demonstrated in the past \cite{30, 31}, provided additivity holds, subsystem mass (particle number) distributions can be determined in the thermodynamic limit directly from the knowledge of only variance of subsystem mass as a function of mass density, irrespective of whether the systems are in or out of equilibrium. Thus additivity could provide a useful simplification in characterizing fluctuations in driven systems as, in that case, macroscopic properties of the systems can be determined solely through the variance of some conserved variables in the systems. However, verifying additivity is not an easy task in general. Of course, additivity can in principle be checked analytically by explicitly calculating steady-state subsystem mass distributions. Though, in most cases, it may not be possible to calculate the exact functional form of the variance, which would be then required to obtain the subsystem mass distribution analytically \cite{30, 31}. As we demonstrate here, this particular difficulty could be bypassed by using a numerical method instead.

In this paper, we characterize, through an additivity property, particle-number or coarse-grained density fluctuations in paradigmatic models of self-propelled particles, namely the Vicsek model and its variants. For simplicity, we consider only the cases when the systems are in an isotropic, and homogeneous, disordered fluid phase, where macroscopic velocity vanishes in the thermodynamic limit. We specifically ask whether particle-number fluctuations in Vicsek-like systems can be described by an intensive thermodynamic variable, analogous to an equilibrium-like chemical potential. We answer the question in the affirmative, by using a computational scheme within additivity. We numerically integrate a fluctuation-response relation - a direct consequence of additivity property, to obtain a nonequilibrium chemical potential and free energy density, which characterize density fluctuations in the systems. By using the above two thermodynamic potentials, we compute log-arithmetic of the probabilities of density large-deviations, also called the large deviation functions, and compare them with that obtained from simulations, by performing a scaling analysis of the subsystem number distributions for various subsystem sizes. We find theory and simulations are in excellent agreement, providing a strong evidence of the existence of an equilibrium-like chemical potential, which governs density fluctuations in the Vicsek-like models of self-propelled particles.

The organization of the paper is as follows. In Sec. \textsection{II} we discuss additivity property and describe the methodology adopted here for numerical computation of subsystem particle-number distributions and density large deviation functions. In Sec. \textsection{III} we present our theoretical and simulation results for three model systems - the Vicsek model in Sec. \textsection{III A} variant I of the Vicsek model in Sec. \textsection{III B} and variant II of the Vicsek model in Sec. \textsection{III C}. Finally, we summarize in Sec. \textsection{IV} with some concluding remarks.

\section{II. Additivity andSubsystem Particle-Number Distribution}

In this section, we discuss, within additivity, the numerical scheme, which is used here to calculate probability distribution of subsystem particle-number. Let us first elucidate additivity property in the context of particle-number fluctuations. We consider a system, consisting of $N$ interacting particles, which are confined in a volume $V$. Importantly, the total particle-number $N$ is conserved in the system. We then divide the system in a large number $\nu = V/v$ of identical subsystems, each having a volume $v$. Provided that the subsystem size $l = v^{1/d}$, $d$ being the dimension, is much larger than the microscopic spatial correlation length in the system, additivity property implies the following. The joint probability distribution $\text{Prob.}\{\{n_k\}\}$ of subsystem particle numbers $\{n_k\}$, with $n_k$ being particle number in $k$th subsystem, has then the following product form \cite{25, 31},

$$\text{Prob.}\{\{n_k\}\} \approx \prod_{k=1}^{\nu} W_v(n_k) Z(N, V) \delta \left( \sum_k n_k - N \right),$$

(1)

in the thermodynamic limit of $N, V \rightarrow \infty$ with global number density $\rho = N/V$ fixed. In the above equation, $W_v(n_k)$ is an unknown weight factor which has to be determined (discussed below), $Z = \sum_{\{n_k\}} \prod_k W_v(n_k) \delta (\sum_k n_k - N)$ is the normalization constant, or the partition sum. Note that, in Eq. 1, the weight factor $W_v(n_k)$ for the $k$th subsystem depends on the particle-number $n_k$ and volume $v$ of the $k$th subsystem only, not on the other subsystems. This particular assumption is nothing but that of a statistical independence, which could emerge on a macroscopic scale, even when there are finite correlations present at the microscopic scales.

Let us denote the subsystem particle-number distribution function as

$$P_v(n) \equiv \text{Prob.}\{n_k = n\} = \sum_{\{n_i\}; i \neq k} \text{Prob.}\{\{n_i\}\},$$

which is the probability that a subsystem, say the $k$th one, of volume $v$ has $n$ number of particles. By using standard statistical mechanics theory of large deviations and additivity property Eq. 1 \cite{27, 31}, subsystem number distribution for $k$th subsystem can be written as

$$P_v(n) \simeq \frac{W_v(n)}{Z(N, V)} \sum_{\{n_i\}; i \neq k} \prod_{i \neq k} W_v(n_i) \delta \left( \sum_{i \neq k} n_i - N + n \right)$$

$$= \frac{W_v(n) Z(N - n, V - v)}{Z(N, V)}.$$  

(2)

One can now expand $Z(N - n, V - v)$ in the leading order of $n$ and obtain, in the thermodynamic limit,

$$P_v(n) \simeq \frac{1}{Z} W_v(n) e^{\mu \rho n},$$

(3)
where

$$\mu(\rho) = \frac{df(\rho)}{d\rho} \tag{4}$$

is a nonequilibrium chemical potential, $f(\rho)$ is the corresponding nonequilibrium free energy density function $f(\rho) = -\lim_{V \to \infty} \ln Z(N, V)/V$ and $Z(\mu, v) = \sum_n W_v(n) \exp[\mu(n)v]$ is the normalization constant. In the above equations, the symbol '≃' means an equality in terms of logarithm $\ln P_v(n)$ of the large-deviation probability, which can be alternatively written as

$$\lim_{v \to \infty} \frac{\ln P_v(n = \hat{n}v)}{v} = -f(\hat{\rho}) + \mu(\rho)\hat{\rho}, \tag{5}$$

where we denote coarse-grained or subsystem density as $\hat{\rho} = n/v$; by definition, average of subsystem density equals to the global density, $\langle \hat{\rho} \rangle = \rho$. For details of the above analysis, we refer to Refs. [15, 30, 31].

The crucial point here is that, using Eqs. (3) and (5), the nonequilibrium free energy density and chemical potential can be determined as a function of number density, by integrating a fluctuation-response (FR) relation between a nonequilibrium compressibility and number fluctuation - a direct consequence [30, 31] of additivity Eq. (1) or, alternatively, Eq. (3) [30, 31] of additivity Eq. (1) or, alternatively, Eq. (3).

$$\frac{d\rho}{d\mu} = \sigma^2(\rho), \tag{6}$$

where the scaled variance $\sigma^2(\rho)$ of subsystem particle-number $n$ in subvolume $v$ is defined as

$$\sigma^2(\rho) = \lim_{v \to \infty} \frac{\langle (n^2) - \langle n \rangle^2 \rangle}{v}. \tag{7}$$

For the proof of Eq. (6) see Ref. [15]. Now the thermodynamic potentials $\mu(\rho)$ and $f(\rho)$ can be readily calculated by integrating Eqs. (8) and (9) with respect to density $\rho$ and are expressed in an integral form as given below,

$$\mu(\rho) = \int \frac{1}{\sigma^2(\rho)} d\rho + c_1, \tag{8}$$

and

$$f(\rho) = \int \mu(\rho)d\rho + c_2, \tag{9}$$

where $c_1$ and $c_2$ two arbitrary constants of integrations. Without any loss of generality, we put $c_1 = c_2 = 0$ or, in other words, we calculate chemical potential $\mu(\rho) = \int_0^\infty 1/\sigma^2(\rho)d\rho$ and free energy density $f(\rho) = \int_0^\infty \mu(\rho)d\rho$ from a reference density $\rho_0$. Finally, the large-deviation probability $P_v(\hat{\rho}) \equiv P_v(n = v\hat{\rho})$ of subsystem density $\hat{\rho} = n/v$, in the limit of $v$ large, can be written as [15]

$$P_v(\hat{\rho}) \simeq \frac{\exp[-v\eta(\hat{\rho})]}{Z(\mu, v)}, \tag{10}$$

with $\mu(\rho)$ being chemical potential of the system at global density $\rho$ and $Z(\mu, v) = \sum_\rho \exp[-v\eta(\hat{\rho})]$ being the normalization constant. Indeed, Eqs. (10) and (11) and (12) can be understood from that the Laplace transform of the weight factor $W_v(n)$ is related to the Legendre transform of free energy density - an immediate consequence of additivity Eq. (1) [15]. Note that, through Eqs. (8) and (9) the large-deviation probability $P_v(n)$ thus has been determined solely in terms of the variance as given in Eq. (7).

What remains now is to explicitly calculate scaled variance $\sigma^2(\rho)$ of subsystem particle number in various models through simulations, which we do next in the following sections. Then, by numerically integrating Eqs. (8) and (9) we compute the subsystem particle-number distribution $P_v(n)$ and the large deviation function and compare them with that obtained from direct microscopic simulations.

### III. MODELS

The model-systems we consider here consist of two dimensional periodic space in....
where, unlike in equilibrium, the probability weights of the microscopic detailed balance are always vanishingly small in the disordered phase, the microscopic detailed balance is still violated, driving the system out of equilibrium. For generic parameter values, the system at long times eventually reaches a nonequilibrium steady state.

CONSEQUENTLY, THE SYSTEMS ALWAYS REMAIN OUT OF EQUILIBRIUM, Detailed balance is violated at the microscopic level. As discussed in the previous section, to check whether the system possesses an additivity property, we require to take into account the magnitude of the macroscopic velocity, characterized by an order parameter, which, in this case, is taken to be the magnitude of the macroscopic velocity of all particles in the system. For simplicity, in this paper we confine our studies to the disordered fluid phase where macroscopic velocity vanishes ($v = 0$). Although the macroscopic velocity is vanishingly small in the disordered phase, the microscopic detailed balance is still violated, driving the system out of equilibrium.

As discussed in the previous section, to check whether the system possesses an additivity property, we require to characterize particle-number fluctuations on the coarse-grained level. To this end, we study subsystem particle-number fluctuations on the coarse-grained level.
number fluctuations as a function of number density. We consider a subsystem of volume $v = l \times l$ with the global density $\rho = N/V$ (or, equivalently, chemical potential) fixed. In our simulations throughout, we keep subsystem and system sizes much larger than microscopic length scale $R$ and subsystem size, respectively, i.e., $R \ll l \ll L$. Although the total number of particles is conserved, particle number $n$, or coarse-grained density $\hat{\rho} = n/v$, in a subsystem fluctuates in time and is a random variable, whose statistics are of our interest here and are presented below.

According to the numerical scheme of Sec. [II], we first calculate in direct microscopic simulations the scaled variance $\sigma^2(\rho)$ [Eq. (7)] of subsystem particle number. In Fig. [I] we plot the scaled variance $\sigma^2(\rho)$ as a function of number density $\rho$ for various values of noise strength, $\eta = 2\pi/3$, $5\pi/6$, $2\pi/3$ and $\pi/2$. For the maximum possible noise strength $\eta > 2\pi$, the system essentially behaves like an ideal gas of noninteracting particles and consequently the scaled variance $\sigma^2(\rho) = \rho$ increases linearly as a function of density $\rho$. [II]. However, for lower noise strength $\eta < 2\pi$, the collective behavior sets in and the scaled variance grows rapidly as a function of density in a highly nonlinear fashion. The scaled variance finally diverges at a critical density, beyond which macroscopic clusters of particles are formed in the system.

Using the above functional dependence of the scaled variance on density, as obtained from simulations (Fig. [I]), we numerically integrate Eqs. (8) and (9), with respect to density $\rho$, to obtain chemical potential and free
energy density, respectively. Then, using Eq. (11), we numerically compute subsystem particle number distribution $P_v(n)$ as a function of subsystem particle number $n$ for various values of global densities $\rho$ and noise strengths $\eta$. We also directly calculate the number distributions $P_v(n)$ from microscopic simulations of the Vicsek model. In Fig. 2 we plot the number distributions $P_v(n)$ as a function of $n$ for three different sets of global density and noise strength: (i) $\rho = 0.1$ and $\eta = 2\pi/3$ (green triangles), (ii) $\rho = 0.1$ and $\eta = \pi/2$ (violet circles) and $\rho = 0.2$ and (iii) $\eta = 2\pi/3$ (yellow squares). We compare the number distributions from simulations with that obtained from additivity theory [Eq. (11)] in Fig. 2 where green, violet and yellow lines represent theoretically obtained number distributions for sets (i), (ii) and (iii) of density and noise strength, respectively. As one can see, theory and simulations are in quite good agreement over several orders of magnitudes of the probabilities; notably, there is no fitting parameter involved in the theory.

Next we perform a scaling analysis to check whether the large deviation probability $P_v(\hat{\rho} = n/v) \sim \exp[-v h(\hat{\rho})]$ or, equivalently, the density large deviation function $-h(\hat{\rho})$, obtained from simulations for different subsystem sizes, converges to that obtained from additivity theory Eq. (12) in the central region, deviate significantly from the Gaussian distributions. Consequently, the corresponding density large-deviation functions have non-parabolic tails, which are remarkably well captured by additivity theory [Eq. (13)].

### B. Variant I of the Vicsek Model

Now we consider a variant of the Vicsek model, which we refer to as variant I, consisting of $N$ particles moving in continuum in a periodic box of volume $V = L \times L$. The variant I is similar to the one introduced previously in Ref. [4], which is different from the original Vicsek model in the way the noise term, i.e., the error in estimating the direction of a particle, is incorporated in the dynamics. The error or the noise is now added separately to each of the components of the direction vector, obtained by averaging over the neighbors within a disk of radius $R = 1$. In other words, the noise term in variant I constitutes

![Image](image-url)
a vector noise, as opposed to the scalar (angle) noise in the Vicsek model. However, apart from the noise term, the deterministic part of the dynamics is the same as in the Vicsek model. The modified equations of motion are given by

\[ \theta_i(t + 1) = \arctan \left( \frac{(\sin \theta_i(t))^R}{(\cos \theta_i(t))^R + \eta \sin \xi_i(t)} \right), \] (15)
\[ \mathbf{r}_i(t + 1) = \mathbf{r}_i(t) + u_0 \cos \theta_i(t + 1), \sin \theta_i(t + 1)), (16) \]

where angular bracket \( \langle * \rangle^R \) denotes average over all neighboring particles \( j \) satisfying \( |\mathbf{r}_j(t) - \mathbf{r}_i(t)| < R = 1 \), \( \xi_i(t) \in [-\pi, \pi] \) is a uniformly distributed random angle, \( \eta \) is the noise strength and \( u_0 = 0.5 \) is the self-propulsion speed of the particles. Total particle number is conserved under the above dynamics and, at long times, the system reaches a nonequilibrium steady state. As in the Vicsek model, beyond a particular value of the density and noise strength, we observe a phase transition from an isotropic disordered fluid phase with vanishing macroscopic velocity (\( v_a = 0 \)) to an ordered phase with nonzero macroscopic velocity (\( v_a \neq 0 \)) \( \mathbb{2}, \mathbb{3} \). The exact nature of the phase diagram for this particular noise variable is not fully understood though \( \mathbb{5} \). For simplicity, we confine our studies to the disordered phase, where the system remains homogeneous and which, due to the violation of detailed balance, is however still out of equilibrium.

To calculate subsystem particle-number distribution within additivity, we first calculate in simulations the scaled variance \( \sigma^2(\rho) \) of subsystem particle number as a function of density \( \rho \). In Fig. 4 we plot \( \sigma^2(\rho) \) as a function of \( \rho \) for various values of the noise strengths \( \eta = 0.4, 0.5, 0.6 \) and 1.0. The scaled variance grows quite rapidly in a nonlinear fashion, except at large noise strength where the particles become noninteracting, leading to the linear dependence of the scaled variance on density, i.e., \( \sigma^2(\rho) = \rho \) as \( \eta \to \infty \) as in an ideal gas. However, for a finite noise strength, the scaled variance diverges beyond a certain density and the system becomes inhomogeneous with macroscopic particle clusters formed in the system.

Next, using the functional dependence of scaled variance \( \sigma^2 \) on density \( \rho \), we numerically integrate Eqs. (11) and (12) to obtain chemical potential and free energy density and to compute probability distribution \( P_v(n) \) of subsystem particle numbers as given in Eq. (11).

We also calculate subsystem number distributions from direct microscopic simulations. In Fig. 3 we plot the number distributions \( P_v(n) \) as a function of subsystem particle number \( n \) for three different sets of global density and noise strength: (i) \( \rho = 0.1 \) and \( \eta = 0.6 \) (green triangles), (ii) \( \rho = 0.1 \) and \( \eta = 0.5 \) (violet circles), and (iii) \( \rho = 0.2 \) and \( \eta = 0.6 \) (yellow squares); we take system size \( L = 500 \). We compare the number distributions in simulations with that computed within additivity using Eq. (12).

As in the Vicsek model, which we refer to as variant II and is similar to variant I, with the two components of the vector noise term however now being independent of each other. The equations of motion are given by

\[ \theta_i(t + 1) = \arctan \left( \frac{(\sin \theta_i(t))^R}{(\cos \theta_i(t))^R + \eta \cos \xi_i(t)} \right), \] (17)
\[ \mathbf{r}_i(t + 1) = \mathbf{r}_i(t) + u_0 \cos \theta_i(t + 1), \sin \theta_i(t + 1)), (18) \]

where \( \xi_i, \xi_i' \) are two statistically independent and identical random angles, uniformly distributed in the range \([-\pi, \pi] \), \( \eta \) is the strength of the vector noise and \( u_0 = 0.5 \) is the self-propulsion speed of the particles. Beyond a critical value of density or noise strength, we observe a phase transition from a disordered fluid phase to an ordered phase, where macroscopic particle clusters form in the system and the macroscopic velocity takes a nonzero value (\( v_a \neq 0 \)). This particular version of the Vicsek model has not been studied before in the literature and the details of the phase diagram will be presented elsewhere \( \mathbb{5} \). In this work, we test additivity in the model circles) and 45 (yellow inverted triangles), respectively. Then we compare in Fig. 6 the large deviation functions with that computed within additivity using Eq. (12). We find theory and simulations are in quite good agreement with each other. Moreover, in the same figure, we compare the large deviation functions, obtained from theory and simulations, with the ones obtained from the Gaussian distributions with mean subsystem particle number \( \langle n \rangle = v_0 \) and variance \( \langle n^2 \rangle - \langle n \rangle^2 = v_0 \sigma^2(\rho) \) (sky-blue lines in Fig. 6). The large deviation functions, beyond the central region around the mean density, deviate significantly from the Gaussian ones (parabolas in Fig. 6).

Indeed, additivity theory captures remarkably well the non-parabolic (non-Gaussian) tails observed in simulations.

C. Variant II of the Vicsek Model

In this section, we consider another variant of the Vicsek model, which we refer to as variant II and is similar to variant I, with the two components of the vector noise term however now being independent of each other. The equations of motion are given by
We first calculate scaled variance $\sigma^2(\rho)$ of subsystem particle number and plot $\sigma^2(\rho)$ as a function of density $\rho$ in Fig. 7 for various noise strengths $\eta = 0.4, 0.5, 0.6$ and 1.0. In the limit of noise strength large, the system behaves like a noninteracting ideal gas; consequently, the scaled variance of subsystem particle number is a linear function of density, $\sigma^2(\rho) = \rho$ as $\eta \to \infty$. However, for a finite noise strength, the scaled variance increases rapidly in a highly nonlinear fashion and, beyond a critical density (depending on the value of noise strength), it diverges as macroscopic particle clusters start forming in the system. Numerically integrating Eqs. 8 and 9 and then using Eq. 11, we also compute particle number distributions $P_v(n)$ for three sets of density and noise strength: (i) $\rho = 0.05$ and $\eta = 0.6$ (green triangles), (ii) $\rho = 0.05$ and $\eta = 0.5$ (violet circles), and (iii) $\rho = 0.1$ and $\eta = 0.6$ (yellow circles). We then calculate number distributions $P_v(n)$ from direct microscopic simulations. In Fig. 8 we plot the number distributions $P_v(n)$ as a function of particle number $n$ and compare them with that in disordered fluid phase, which, due to violation of detailed balance, remains out of equilibrium.
We compare the density large deviation functions, (theory and simulations) with the Gaussian ones (parabolas, sky-blue lines in Fig. 9), obtained from the Gaussian distributions \( \sim \exp\left[-v\left(\rho - \rho^\ast\right)^2/2\sigma^2(\rho)\right] \) with mean \( \rho^\ast \) and variance \( \sigma^2(\rho) \). Clearly, the actual number distributions deviate significantly from the Gaussian distributions. Consequently, the large deviation functions (number distribution) have non-parabolic (non-Gaussian) tails, which are indeed well captured by additivity theory.

### IV. SUMMARY AND CONCLUDING REMARKS

In this paper, we study coarse-grained density fluctuations in the paradigmatic models of self-propelled particles or active matters, which are inherently driven out of equilibrium through a mechanism of self-propulsion of the constituent particles. We consider a broad class of self-propelled particles with alignment interactions, namely the Vicsek models and its variants. The systems consist of particles, which are point-like, have random propulsion velocities, and move in continuum on a two-dimensional periodic space. Particles interact among each other through alignment interactions: At any instant, particles try to follow their neighboring particles in a way so that they align themselves, and move, along a direction, which is obtained by averaging over instantaneous velocities (or directions) of their neighbors. At long times, the systems eventually reach a nonequilibrium steady state.

We coarse-grain a system by dividing the system into many subsystems and characterize subsystem particle-number (or coarse-grained density) fluctuations through an additivity property, which leads to a remarkable large-scale thermodynamic structure for the Vicsek-like systems. By using a fluctuation-response relation - a direct consequence of additivity property and employing a numerical scheme developed in this work, we compute the large-deviation probabilities of subsystem particle number, and the corresponding density large-deviation functions in the disordered fluid phase, where macroscopic velocity vanishes in the thermodynamic limit. It should be noted that, though there is no macroscopic current in the disordered phase, the systems still remain out-of-equilibrium, due to the violation of detailed balance, and their microscopic probability weights thus cannot be described by the equilibrium Boltzmann-Gibbs distribution.

We compare the density large deviation functions,
FIG. 9: Variant II. Large deviation function $-h(\hat{\rho}) = \ln[\mathcal{Z}(\mu, \nu)P_\nu(\hat{\rho} = n/v)]/v$ [Eq. (12)] is plotted as a function of coarse-grained subsystem density $\hat{\rho} = n/v$, with $n$ and $v$ being subsystem particle-number and subvolume, respectively, for various subsystem sizes $v = l \times l$ with $l = 30$ (violet squares), 35 (green triangles), 40 (sky-blue circles), 50 (yellow inverted triangles) for three sets of noise strength and global density - (i) $\eta = 0.5$ and $\rho = 0.05$ (first panel), (ii) $\eta = 0.6$ and $\rho = 0.05$ (second panel) and (iii) $\eta = 0.6$ and $\rho = 0.1$ (third panel). Points - simulations, red lines - additivity theory, sky-blue lines - parabolic (due to Gaussian distributions) large deviation functions. Note that non-parabolic tails (due to non-Gaussian number distributions) are well captured by theory.

computed within the theory of additivity, with those obtained from direct microscopic simulations of the models; theoretical and simulation results are found to be in excellent agreement over several orders of magnitude of the large-deviation probabilities of coarse-grained density, without any fitting parameters involved in the theory. Notably, the subsystem particle-number distributions (equivalently, the density large deviation functions) have non-Gaussian (non-parabolic) tails, which are quite well captured by additivity theory. Our results strongly suggest that coarse-grained density fluctuations in self-propelled-particle systems with Vicsek-like interactions are governed by a nonequilibrium chemical potential and a corresponding free energy function.

There are a few remarks in order. In equilibrium systems with short-ranged interactions in the Hamiltonian, the Boltzmann-Gibbs probability weights of microscopic configurations immediately imply additivity [35]. On the other hand, not much is known about the microscopic structure of systems having a nonequilibrium steady state, which cannot be associated with a Hamiltonian as such. Interestingly, the Boltzmann-Gibbs distribution, though sufficient, is not necessary for additivity to hold [28, 31]. However, determining the precise conditions, for which additivity would hold in nonequilibrium and a steady-state thermodynamics could be constructed, is a nontrivial problem [34, 35] and yet to be done [36]. In this scenario, it would be indeed worth checking case-by-case whether a certain class of nonequilibrium systems could possess an additivity property.
However, in most cases, an analytic expression of the variance of subsystem mass (particle-number) as a function of mass density cannot be obtained and the task of verifying additivity in nonequilibrium systems is not easy. We provide here a simple computational scheme, which could help one to compute density large-deviation functions, and thus to test additivity, in a driven system. In the light of our work, we believe additivity could prove to be a useful concept in characterizing fluctuations not only in systems with Vicsek-like interactions, but also in other active-matter systems.

Moreover, our work brings to the fore some interesting open issues, studies of which could provide further insights into the large-scale properties of self-propelled particles in general. Firstly, it remains to be seen whether additivity can be used to characterize properties of Vicsek-like systems near and above criticality, e.g., in the ordered phase, which is known to exhibit giant number fluctuations. Secondly, so far we have studied only the static structure of Vicsek-like systems, such as particle-number fluctuations, and have shown that the number fluctuations are related to a nonequilibrium compressibility, through a fluctuation-response relation - reminiscent of fluctuation-dissipation theorems in equilibrium. However, the interplay between static and dynamic structure, which possibly play an important role in the large-scale behaviors of self-propelled particles, has not been investigated in this work. Indeed, unlike in equilibrium, and except in some simple nonequilibrium processes, there is no general theoretical understanding of a possible connection between transport and fluctuations in driven many-particle systems. In this context, exact calculations of various transport coefficients can certainly provide some insights into the collective behaviors of self-propelled particles in general. While it may be quite challenging to calculate transport coefficients in continuum systems, the problem is presumably simpler for systems on a lattice and worth pursuing in future.

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