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Order–Disorder Phase Transition in Heterogeneous Populations of Self-propelled Particles

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Abstract Biological systems are typically heterogeneous as individuals vary in their characteristics, their response to the external environment and to each other. For example, cell diversity plays a crucial role in the successful survival of many biological systems. Phenotypic heterogeneity is associated with cellular response to intercellular communications, the response to external environmental cues, motility modes, and proliferation rates. Here we study the effect of phenotypic diversity on the properties of collective motion in the context of the scalar noise model of collective migration. For simplicity, we study a population that is composed of two sub-populations, each with different sensitivities to external noise. We find that the two sub-populations interact non-additively: Within a large range of parameters, the dynamics of the system can be described by an equivalent homogeneous system with an effective temperature that depends on the average circular mean of the phenotypes. However, if one of the sub-populations is sufficiently "cold", it dominates the dynamics of the group as a whole.

Keywords Collective motion · Self propelled particles · Heterogeneous populations · Order–disorder phase transition

1 Introduction

Complex systems, in particular biological systems, are typically heterogeneous as individuals have disparate characteristics and vary in their properties. In some examples, variations in

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properties average out and do not have any significant effect on the macroscopic properties of the system. However, in many other cases diversity can have a pivotal effect on the system dynamics. For example, it was shown that size variation in excited granular material can lead the system to separate according to size. The impact of heterogeneity on the properties of collective motion, in particular on the order–disorder phase transition, has not been thoroughly studied. Within the context of simplified models of self-propelled particles addressing the general and broad description of the dynamics, most models focus on homogeneous system. That is, it is assumed that all the agents have the same properties and follow the same "rules of engagement" [1]. Notable exceptions are introduction of leaders [2] which creates an expected bias towards the leading population, variability in speed [3], which was found to only affect the rate of convergence to a stationary distribution but not the distribution itself, and variable interactions between two sub-populations [4].

In this paper, we study the effect of heterogeneity in the context of the well-studied scalar noise model (SNM), proposed by Viscek et. al. [5,6]. In this model, N particles move with constant speed v in a rectangular two-dimensional domain $[0, L]^2$ with periodic boundary conditions. Every simulation time step, each particle aligns its direction with the average direction of all particles within an interaction distance R and makes a random turn. In [6], the random turn is taken to be uniformly distributed in a fixed range $[-\eta, \eta]$ for some fixed $\eta \in [0, \pi]$. It is shown numerically that the system undergoes a phase transition between an ordered phase at low temperature/high density and a disordered phase at high temperature/low density. Various aspects of the transition have been studies in the rapidly expanding literature on the SNM and its many variants. For recent reviews see [1,7].

Phase transitions are typically characterized by the scaling of an order parameter - the norm of the average velocity in the case of SNM - close to a critical density $\rho = N/L^2$ or critical temperature. As density is an extensive global parameter, it cannot be directly related to the properties of individuals. On the other hand, temperature is clearly related to, loosely speaking, the "amount of noise in the system", which is characterized by η - a property of individuals. This motivates us to examine a mixed population of particles, each with a different noise parameter. For simplicity, we consider a binary mixture, in which a fraction f_1 of the particles have noise $U(-\eta_1, \eta_1)$, while a fraction $f_2 = 1 - f_1$ have noise $U(-\eta_2, \eta_2)$, where $U(a, b)$ denoted the uniform distribution in (a, b).

The layout of the paper is as follows. Section 2 details the model and discusses the notion of temperature in the context of SVM. We found that it is essential to select the proper measures associated with the statistics of the order parameter for comparing the behaviors of homogeneous populations vs. heterogeneous ones, Sect. 3 presents our main results. In particular, we demonstrate numerically that parameter variability has a non-additive effect which *promotes order* in the sense that a heterogeneous population can be in the ordered phase while a homogeneous one with the same temperature is disordered. We conclude in Sect. 4.

2 The Scalar Noise Model

Consider N particles moving in a rectangular two-dimensional domain $[0, L]^2 \subset \mathbb{R}^2$ with fixed speed v. Let x_i^k denote the position of particle i at time k and $\hat{h}_i^k$, the normalized "head direction", $|\hat{h}_i^k| = 1$. For convenience, we denote the angle between $\hat{h}_i^k$ and the x-axis θ_i^k, $\hat{h}_i^k = (\cos\theta_i^k, \sin\theta_i^k)$. The N particles are divided into two sub-species: Particles $1 \ldots N_1$ are species 1, while particles $N_1 + 1 \ldots N$ are species 2. Let p_i denote the species index of

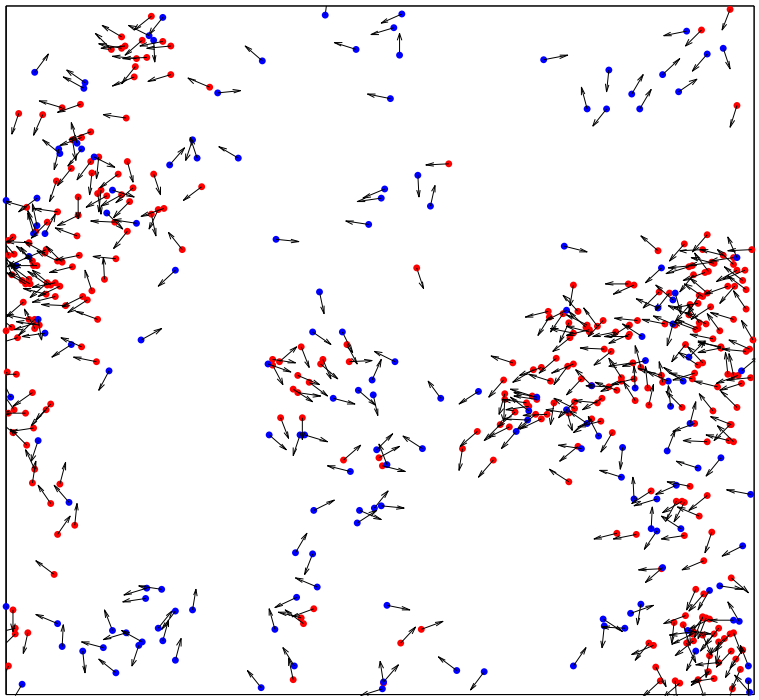

Fig. 1 A snapshot from a simulation with 500 particles (Color figure online)

particle i, $p_i = 1$ for $i = 1, \ldots, N_1$ and $p_i = 2$ otherwise. We consider a discrete dynamical system which evolves according to the following rules (preformed synchronously and in order)

1. Advance: $x_i^{k+1} = x_i^k + v\hat{h}_i^k$.
2. Align:

$$\tilde{h}_i^{k+1} = \frac{1}{n_i^k} \sum_{j \in A_i^k} \hat{h}_j, \tag{2.1}$$

   where $A_i^k = \{j : |x_i^k - x_j^k| \leq R\}$, the set of neighbors of i at time k within an interaction distance R and $n_i^k = |A_i^k|$ is the number of neighbors.
3. Random turn: Rotate $\tilde{h}_i^{k+1}$ by a random angle and normalize. Specifically, let α_i^k denote a random angle, uniformly distributed in $[-\eta_{p_i}, \eta_{p_i}]$, $\alpha_i^k \sim U(-\eta_{p_i}, \eta_{p_i})$. Then, $\hat{h}_i^{k+1} = h_i^{k+1}/|h_i^{k+1}|$, where

$$h_i^{k+1} = \begin{pmatrix} \cos\alpha_i & -\sin\alpha_i \\ \sin\alpha_i & \cos\alpha_i \end{pmatrix} \tilde{h}_i^{k+1}. \tag{2.2}$$

With $\eta_1 = \eta_2$, the model reduces to the standard SNM described in [6]. Figure 1 shows a snapshot from a simulation with 500 particles. Parameters are $f_1 = 2/3$, $f_2 = 1/3$, $\eta_1 = \pi/3$, $\eta_2 = 2\pi/3$, $R = 1$, $\rho = 2$ and $v = 0.1$.

With random initial conditions (uniform spatial distribution and uniform angles), the system relaxes into a steady state that can be characterized by an order parameter, which is the norm of the average head direction

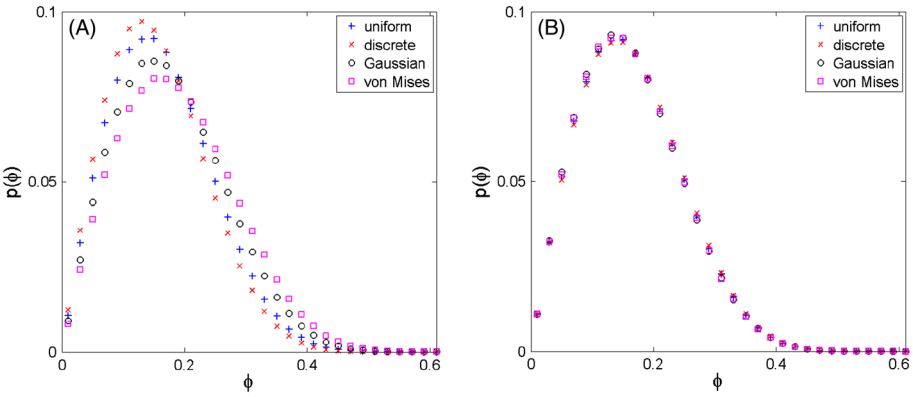

Fig. 2 The distribution of ϕ with different choices of noise. **a** All noise distributions have the same variance. **b** All noise distributions have the same circular mean (Color figure online)

$$\phi^k = \left| \frac{1}{N} \sum_j \hat{h}_j^k \right|. \tag{2.3}$$

We will also be interested in the average order parameter $\phi = \langle \phi^k \rangle$, where $\langle \cdot \rangle$ denotes averaging with respect to all time steps, all particles and possibly repeated simulations.

The choice of uniformly distributed random turns seems arbitrary. Indeed, other choices have been used in the literature such as Gaussian or the von Mises distribution [8–11]. The latter is the maximum entropy distribution for a given circular mean, and is described by the probability density $p(\alpha) = \exp(\kappa \cos(\alpha - \mu))/(2\pi I_0(\kappa))$, where $I_0(z)$ is the zero'th order modified Bessel functions of the first kind. The parameter μ is the average angle and $1/\kappa$ is related to the variance. Figure 2a shows the distribution of ϕ^k obtained for a homogeneous population ($\eta_1 = \eta_2 = \eta$) with four different choices of distributions for the random turning angles: uniform distribution, Gaussian, Bernoulli ($\pm\eta$ with equal probability) and von Mises (with $\mu = 0$). Parameters were chosen so that all distributions have the same variance. Clearly, the steady state depends on the choice of noise. Instead, one should consider circular statistics [10]. Let α denote a real random variable. The circular mean of α is defined as

$$\mathbb{E}[e^{i\alpha}] = \mathbb{E}[\cos\alpha] + i\mathbb{E}[\sin\alpha]. \tag{2.4}$$

To resolve the issue studied here (homogeneous vs. heterogeneous populations), we focused on distributions that have even densities, hence, the imaginary part vanishes. For example, with a uniform distribution $\alpha \sim U[-\eta, \eta]$, we have that

$$\mathbb{E}[e^{i\alpha}] = \int_{-\eta}^{\eta} p(\alpha) e^{i\alpha} d\alpha = \int_{-\eta}^{\eta} \frac{1}{2\eta} (\cos\alpha + i \sin\alpha) d\alpha = \mathrm{sinc}(\eta).$$

Indeed, Fig. 2B shows the distribution of ϕ for the same four distributions with parameters chosen such that all distributions have the same circular mean. The steady states are equivalent up to statistical error. To this end, we use the circular average to define the temperature as follows

$$\begin{aligned} T_1 &= 1 - \mathrm{sinc}(\eta_1) \\ T_2 &= 1 - \mathrm{sinc}(\eta_2) \\ T &= f_1 T_1 + f_2 T_2. \end{aligned} \tag{2.5}$$

We note that T is in [0, 1] and is increasing with increasing noise.
The circular mean is also related to the average order parameter. Denote

$$\beta_i^k = \theta_i^{k+1} - \theta_i^k. \tag{2.6}$$

In words, β_i^k is the change in direction particle i makes following step k, including both alignment and random turning. Therefore, $\cos\beta_i^k$ is the projection of the new direction on the previous one. In particular, suppose the system is perfectly aligned, $\phi^k = 1$. After a single step $\phi^{k+1} = (1/N)\sum_j \cos\beta_j^k$, i.e., the average turn. Hence, $\phi = \langle\cos\beta_i^k\rangle$ is the observed circular mean. This identity is confirmed in simulations, see also [12]. The difference between the observed circular mean $\phi = \langle\cos\beta_i^k\rangle$ and the circular mean of the random turns is always negative since alignment decreases the spread of angles.

3 Results

The main objective of the paper is a systematic comparison between the physical properties of homogeneous systems ($T_1 = T_2 = T$) and heterogeneous ones ($T_1 \neq T_2$), having the same overall temperature T. In particular, we are interested in finding the effect of heterogeneity on the critical temperature at fixed concentrations.

Numerically, one of the most precise methods for detecting the critical temperatures is by comparing the Binder cumulant at different temperatures and concentrations [11–13]. However, with heterogeneous populations such a comparison is not trivial since, due to finite size fluctuations, the location of the critical point may not be the same along different cuts in the $T_1 - T_2$ plane. For this reason, we will consider a different measure that qualitatively distinguishes between ordered and disordered systems. Consider the location of the maximum in the distributions (the mode) of the order parameter described in Fig. 3. With a low

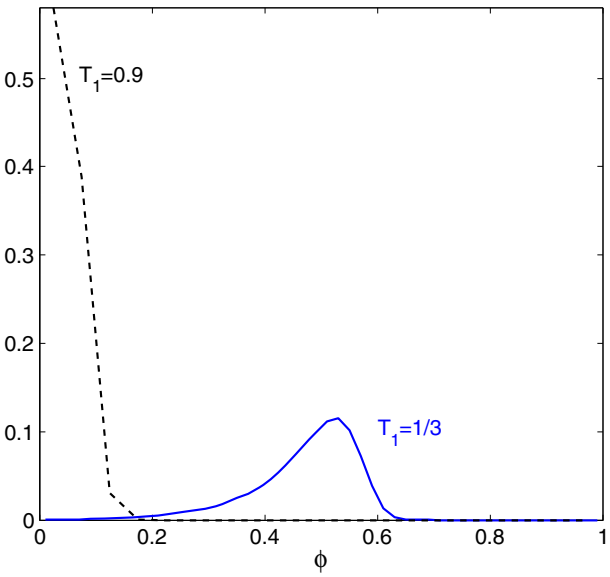

Fig. 3 The steady state distribution of the order parameter ϕ. $T_2 = 2/3$ (Color figure online)

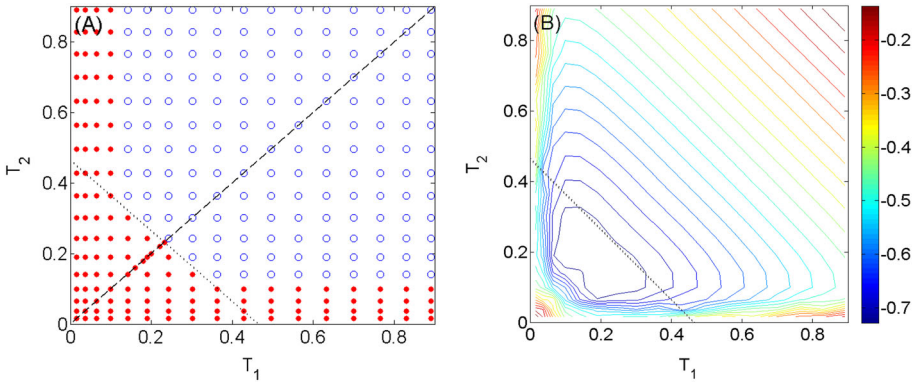

Fig. 4 A heterogeneous system with 50,000 particles at $f_1 = f_2 = 1/2$. **a** The phase diagram. *Red dots* indicate an ordered phase, while *blue circles* are disordered. **b** The difference between the observed circular mean ϕ and the circular mean of the random turns $1 - T$. Up to statistical error, if T_1 or T_2 are small enough, level *curves* are close to *horizontal* or *vertical lines*. Otherwise, they are *diagonal lines*, indicating a constant temperature. The *dashed curve* shows the homogeneous $T_1 = T_2$ line. The *dotted line* is the constant temperature curve passing through the homogeneous critical temperature (Color figure online)

temperature (solid blue curve), the mode is around $\phi = 0.5$. However, when the temperature is high enough (dashed black curve), the density is monotonically decreasing and the mode is at $\phi = 0$. A non-monotone density is typically associated with increased kurtosis, which is, up to a constant, the Binder cumulant. Accordingly, we will refer to the case in which the mode is strictly positive (more precisely, larger then $2/\sqrt{N}$) as the ordered phase. Otherwise, we will refer to it as disordered.

Figure 4a shows the phase diagram of a symmetrically mixed population ($f_1 = f_2 = 1/2$) as a function of T_1 and T_2. Red points indicate a system in the ordered phase (mode > 0) while blue points indicate a disordered phase. The dashed diagonal line is the homogeneous $T_1 = T_2$ case. As a reference, Fig. 5 shows the phase diagram of the same 2-population mixtures when the two populations are not interacting. In this simple case, the system is in the ordered phase only if both sub-populations are ordered. However, when the two populations are interacting, it is evident that heterogeneity has a non-trivial effect on the steady state. In particular, if one of the species is "cold enough" (either T_1 or T_2 are below approximately 0.25), then the system is ordered. Note that this does not correspond to the critical temperature of a single species on its own, which is slightly higher (0.33). At intermediate temperatures the ordered–disordered transition occurs close to the dotted line which indicates the $f_1 T_1 + f_2 T_2 = T_{\text{critical}} = 0.36$ curve. Figure 4b shows the level curves of

$$\psi(T_1, T_2) = \phi(T_1, T_2) - T - 1 = \langle \cos \beta_i^k \rangle - \langle \cos \alpha_i^k \rangle. \tag{3.1}$$

Recall that the first is the real part of the circular mean of turns as observed in simulations, i.e., including both random turns and orientation interaction. The second term is the real part of the circular mean of random turns alone. As discussed above, ψ is always negative. Similar to the phase diagram, if either T_1 or T_2 are sufficiently small, then the level curves of ψ are close to horizontal or vertical lines, indicating that the colder population dominates. Otherwise, the level curves have slope -1, which implies that ψ is constant at constant temperature $T = (T_1 + T_2)/2$. Similar behavior can be observed in Fig. 6 with $f_1 = 3/4$, showing an expected bias towards the first population. Simulation parameters are $N = 50000$, $v = 0.1$, $R = 1$, $\rho = 0.6$. Every point in Figs. 4, 5 and 6 was obtained by averaging ten simulations,

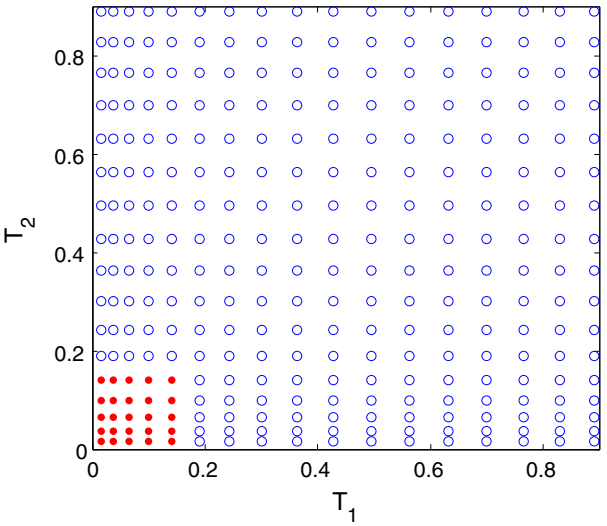

Fig. 5 The phase diagram with a mixture of non-interacting systems. All parameters are the same as in Fig. 4. The system is in the ordered phase only if both populations are sufficiently cold (Color figure online)

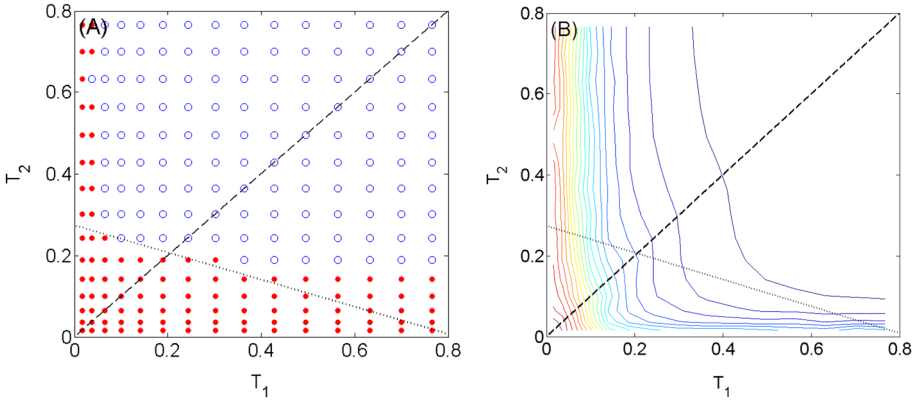

Fig. 6 A heterogeneous system with 50,000 particles at $f_1 = 3/4$, $f_2 = 1/4$. **a** The phase diagram. *Red dots* indicate an ordered phase, while *blue circles* are disordered. At intemediate temperatures, the transition is close to a line with slope $-1/4$ passing through $T_1 = T_2 = T_{\text{critical}}$, the critical temperature of a homogenuous system. **b** The difference between the observed circular mean ϕ and the circular mean of the random turns $1 - T$. Up to statistical error, if T_1 or T_2 are small enough, level *curves* are close to *horizontal* or *vertical lines*. The *dashed curve* shows the homogeneous $T_1 = T_2$ line. The *dotted line* is the constant temperature curve passing through the homogeneous critical temperature (Color figure online)

each consisting of 10^5 steps. Simulations with a larger N did not change these observations (up to statistical errors). However, the critical temperature does weakly depend on N.

The spatial distribution of particles can be observed by analyzing the radial distribution function of each of the species, See Fig. 7. Simulation parameters are the same as in Fig. 2. Surprisingly, we find that on average, heterogeneous systems are slightly less clustered and more dispersed.

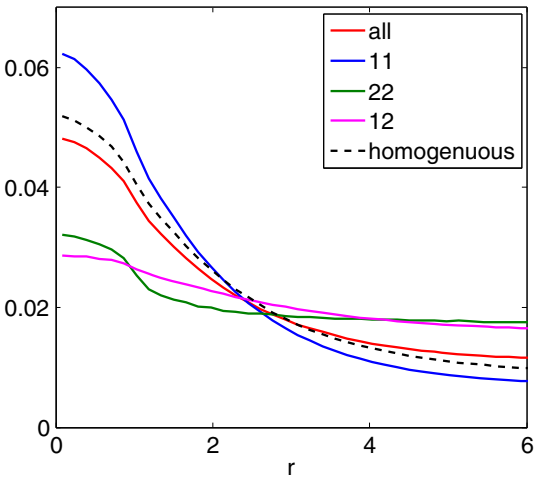

Fig. 7 Radial distribution functions. Solid curves show the heterogeneous case: between a test particle and all other particles (*red*), between a test particle of species 1 and all other species 1 particles (*blue*), between a test particle of species 2 and all other species 2 particles (*green*) and between a test particle and all other particles belonging to the other species (*purple*). The *dashed curve* shows the radial distribution function of a homogeneous system with the same temperature (Color figure online)

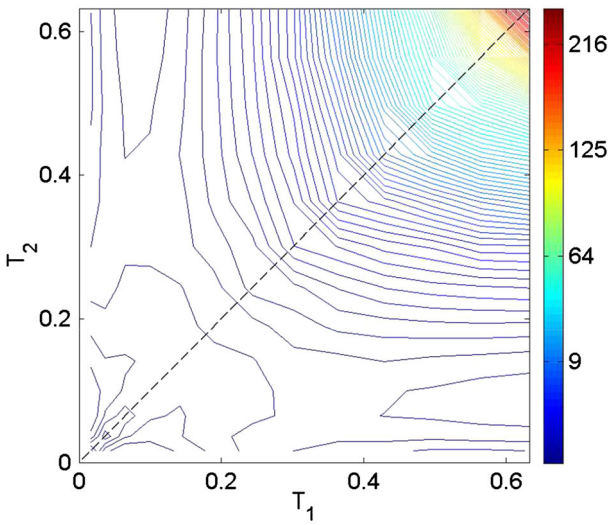

Fig. 8 The characteristic convergence time to the steady state (Color figure online)

Finally, the rate of convergence to the steady state also depends non-trivially on parameter variability. Figure 8 shows the level curves of the characteristic convergence time as a function of T_1 and T_2. Simulation parameters are $N = 100$, $f_1 = f_2 = 1/2$, $v = 0.1$, $R = 1$ and $\rho = 0.3$. Each point in Fig. 8 consists of 50,000 simulations with different number of steps. At each simulation length, the empirical distribution of ϕ was evaluated until it became approximately stationary. The L_2 distance between the distribution of ϕ after a fixed number of steps and the steady state decay exponentially. Convergence rates were obtained by a linear least squares fit to a semi-log plot (not shown).

To further quantify the interaction between the two populations we examine the dynamics of one population in the effective mean field of the second as follows. First, we simulate a small system and estimate the average order parameter of each population,

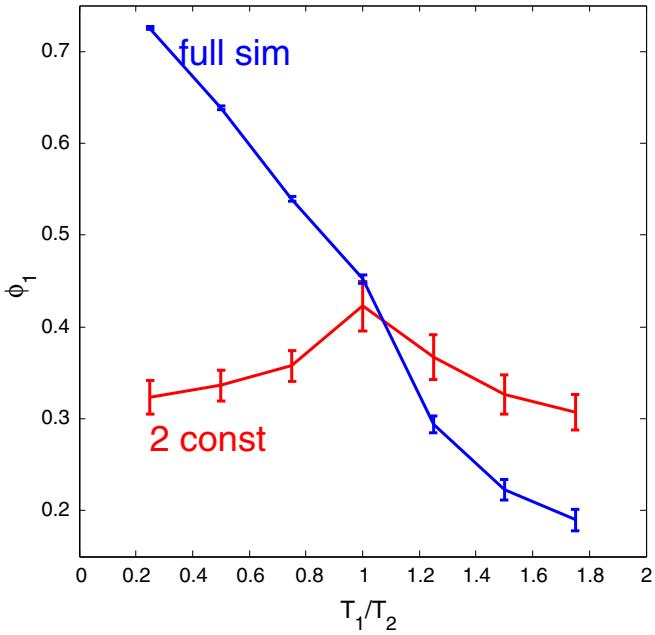

Fig. 9 The dynamics of one population in the presence of an effective second population as a function of T_1/T_2. The *curve* denoted 'full sim' is the full simulation of the SVM described in Sect. 2. The *curve* denoted '2 const' was generated by holding the head direction of the second population fixed with circular variance ϕ_2 obtained by the full simulation. *Error bars* show the standard deviation (Color figure online)

$$\phi_i = \left\langle \frac{1}{N_i} \sum_{p(j)=i} \hat{h}_j^k \right\rangle , \quad i = 1, 2 \tag{3.2}$$

Next, we repeat the simulation, holding the head directions of population 2 fixed. Initial conditions of population 2 are such that the circular mean of all species 2 particles is ϕ_2 as found in the full simulation. In other words, we fix population 2 to have the effective circular mean observed in the full simulation, including both orientation interactions and noise, and study its effect on population 1. The difference is the absence of feedback as species 2 does not respond to the dynamics of species 1. Figure 9 shows the average of ϕ_1 as a function of T_1/T_2. When $T_1 = T_2$, the interaction of population 1 with the fixed population 2 yields the same average as the full simulation. However, if T_1 is different than T_2, then the two populations interact in a non-trivial manner, which cannot be described with a mean-field theory. Simulation parameters are $N = 500$, $R = 1$, $v = 0.05$, $\rho = 0.2$, $T_2 = 0.2$ and $f_1 = f_2 = 0.5$. Averages were obtained by running 2,000 simulations, each with 10^5 steps.

4 Conclusion

Phenotypic heterogeneity plays an important role in cooperative survival strategies, as it renders the population more adaptable to a wide range of environmental conditions. In this paper, we demonstrated that variability in the movement characteristics among individuals can lead to macroscopic effects in groups of moving individuals. It is expected that leaders [2],

experts [14], or individualists [15], can naturally push the system towards a more ordered state. However, our results show that simply by allowing particles to have different characteristics can lead to a collective effect and induce collective motion. Intuitively, once one of the populations is cold enough to cluster and form some collective motion on its own, the other, noisier population can aggregate around areas of coordinated motion. By observing the radial distribution functions, Fig. 7, we see that with a mixed population the range of correlations between the two species is longer than in homogeneous systems. This, in turn, increases the overall consensus and synchronization in the system.

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