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MONTE CARLO SIMULATION ON THE PHASE TRANSITION OF ANIMAL GROUP: A *q*-STATE POTTS MODEL

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Abstract. *We study in this work the phase transition behaviour of animal groups. We assume that the individuals in the group have two classes of state. One is the internal state which can be either excited or non-excited. The other one is characterized by their orientation or direction of motion, it is so called the external state. The internal state plays an important role in the rules of interaction between the individuals. The system is put under a source of external perturbation called "noise", the individuals can freely move from one site to another site on a two-dimension triangular lattice. We use the Monte-Carlo simulation technique for studying the behavior of the model with varying noise. For simplicity, we consider the orientation of individuals which has q states as in the Potts model. We show that the system has three phases which correspond to the uncollected, flocking and runaway behaviors at very low, medium and high noise, respectively. These phases are separated by two first-order transitions.*

Keywords: collective behavior, phase transition, Monte-Carlo simulation, q-state Potts model.

I. INTRODUCTION

The collective behavior is a widely observed phenomenon in various of biological species. In particular the flocking behavior of animal groups. It is one of the main topics which have been extensively investigated during the last two decades using biological, mathematical and physical models. Well-known examples are found in populations such as large schools of fish, the gatherings of birds, the swarming of ants and the herding of sheep [1–5]. The flocking is a behavior of some animal species where they stay together in a group for social reasons. They derive many benefits from these behaviors including defence against predators, easier to move, enhanced foraging success and higher success in finding a mate. Many animal species do not need a leader or an external stimulus to avoid splitting up, move cohesively and adopt a common direction. Therefore, the behaviour of these animal groups can be described by a self-organized system.

Reynolds first suggested a simple model consisting of three rules: separation, alignment, and cohesion rules [6]. These rules describe the behavior of each individual in interaction with other neighboring individuals. A mathematical model is proposed by Cucker and Smale [7] (CSM) using the equations of classical mechanics. In which, the interaction is introduced in the form of attraction or repulsion force which depends on the distance between each individual and its neighbors. However, the equation of motion in CSM is a discrete function of distance [8–10]. On the other hand, T. Vicsek *et al.* introduced a physical model [11] which has been extensively developed during the last 20 years [12–14]. This model is a novel type of dynamics in order to investigate phase transition in non-equilibrium systems based on the ferromagnetic spin model. In which, the velocity and direction of the particles is determined by a simple rule: at each time step, a given particle moves with a constant velocity, a new direction is obtained by the average direction of all the neighborhood particles within a circle of radius R with including a random noise. The effects of vision angle on the phase transition has been investigated [15], the simulation result showed that the schooling behavior is only for the prey species, but not for the predator species. However, all above models are applicable to study the phase transition at high noise only, where the system is changed from the ordered phase to the disordered phase.

In order to study the phase transition behavior of animal group at low noise, a combined model has been introduced with adding the chemical and Morse potentials into the Hamiltonian [16]. The simulation results clearly shown two transitions at very low noise and at high noise. The disadvantages of the model are the complexity of the interaction rules and the high degeneracy configuration of the XY spins. For developing the model, we propose in this paper a new rule of the interaction between two individuals which depends on their internal states. Moreover, we assume that the individuals have only q moving directions (or q orientations), they are defined as q-state in the Potts model. So, the orientation of each individual characterizes to its external state. We perform the simulations by using both standard Monte-Carlo (MC) and multiple histogram (MH) methods. We obtained the order parameter and the concentration as a function of external noise. The results show the existence of three phases which are equivalent to the uncollected, flocking and runaway behaviors of animal group. However, the histogram shows a double peak at both transitions that indicates a signature of the first-order transition.

The paper is organized as follows, Section II is devoted to the description of the model. Section III shows the phase transition behaviors obtained by the simulations. Concluding remarks are given in Sec. IV.

II. THE MODEL

In biology, all the members of an animal group are spread to find foods if there is no danger. In this situation, they are distributed in the space with a small concentration and out of alignment. So, we say the group of animals is in a "uncollected" behavior. When the animals are faced with danger such as predators, they bind together in a small area for safety with the same orientation and high concentration. This state is called "flocking" state. Facing a danger, animals will move away from the predator in the same direction and then stampede as fast as they can when being under the predator's attack. At the final stage, they are in a "runaway" state. In a ferromagnetic spin model, the ordering of a system is quantified by the order parameter or magnetization. The system is in the ordered phase when almost of spins have the same orientation, then the order parameter reaches to maximum. Whereas, when the orientation of the spins are different, therefore the order parameter is about zero and the system is in the disordered phase. The concentration is defined as the amount of spins per unit volume.

In order to study the phase transition behavior, we have to map the group of animals into a physical system. We consider the animal as a particle i with two degrees of freedom: one is an external parameter σ_i characterizing the animal orientation, and the other one is the internal parameter S_i indicating either it is in the non-excited ($S_i = 0$) or in the excited state ($S_i = 1$). The internal individual state is defined with the help of two Ising spins for each animal: the animal is in the internal excited state if its two spins are antiparallel. It is in the non-excited state if its spins are parallel. There are thus $n = 2N$ spins with N being the number of animals in the system. In the absence of an external noise (or the temperature in statistical physics), the system of internal $2N$ Ising parameters S_i is in the disordered phase if these spins are randomly anti-parallel, then we say the internal state is excited. Otherwise, the internal state is non-excited with two parallel spins in each animal. Total number of "up" spins in Ising model could be evaluated by [17]:

$$n_{\uparrow} = \frac{n}{1+\exp(-2\varepsilon/\xi)}, \tag{1}$$

where $\varepsilon > 0$ is the energy of a spin and ξ is the external noise. Hence, the number of down spins is $n_{\downarrow} = n - n_{\uparrow}$. For simplicity, we assume that n Ising spins are randomly distributed on N individuals by an uniform distribution. Denote by N_0 the number of non-excited individuals:

$$N_0 = \frac{n_{\uparrow} - n_{\downarrow}}{2} = \frac{2n_{\uparrow} - n}{2} = n_{\uparrow} - N = N \tanh(\varepsilon/\xi). \tag{2}$$

Thus the number of excited individual is $N_e = N - N_0$. Note that when $\xi \to 0$, $n_{\uparrow} \to n$ or $N_0 \to N$, namely all animals are non-excited. At high noise, $n_{\uparrow} \to n/2$ or $N_e \to N$, so that all animals are excited.

Now, we put this system of individuals on the lattice where each individual can move on 2D triangular lattice of linear size L. The number of lattice sites should be greater than that of individuals, i.e., $L^2 \gg N$. We denote by σ_i the orientation of individual S_i: σ_i is defined as in a q-state Potts model, i.e. $\sigma_i = 1, 2, \ldots, q$. In this model, we consider the case $q = 6$, so the orientations $\sigma_i = 1, 2, \ldots, 6$ of individual S_i can be defined by the vectors which connect a site to its nearest neighbors (NN) with the following angles measured from the x axis: $\varphi_i = 0, \pi/3, \ldots, 5\pi/3$. The interaction between two individuals is given by the Hamiltonian

$$\mathscr{H} = \sum_{<i,j>} K_{i,j} \cos[\pi(\sigma_i - \sigma_j)/3], \tag{3}$$

where the sum $\sum_{<i,j>}$ is made over the third nearest neighboring individuals S_i and S_j. $K_{i,j}$ has a form of Lennard-Jones potential:

$$K_{i,j} = 4J_{i,j}\left[(r_0/r_{i,j})^{12} - (r_0/r_{i,j})^6\right],$$

with $r_{i,j}$ is the distance between two individuals, we choose $r_0 = 0.89$ in order that $K_{i,j} \simeq J_{i,j}$ at $r_{i,j} = 1$. $J_{i,j}$ is the exchange interaction between two individuals which depends on their internal state: $J_{i,j} = 0$ if both individuals are non-excited $S_i = S_j = 0$, and $J_{i,j} = J > 0$ if otherwise.

Let us explain the biological meaning of the Hamiltonian (3). The Lennard-Jones potential is an attractive interaction for long range of distance between the individuals, it helps to the animals moving close to each other. Otherwise, it is a strong repulse interaction for short range of distance, so the individuals are not be curdled. $\cos[\pi(\sigma_i - \sigma_j)/3]$ is the exchange interaction for the alignment of the individuals, thus they have the same orientation in the flocking state.

The main physical quantities such as the order parameter Q and the concentration ρ are defined by

$$Q = \frac{q}{N(q-1)}\sum_{i=1}^{N}(\sigma_i^{\max} - N/q), \tag{4}$$

$$\rho = \frac{1}{N}\sum_{i=1}^{N} n_i, \tag{5}$$

with $q = 6$ and $\sigma_i^{\max} = \max\left(\sum_i \sigma_i\right)$. n_i is the number of NN individuals around S_i.

Let us adopt the following notations. The ordering of the system is quantified by the order parameter Q. When the individuals have different orientations, the order parameter $Q \approx 0$, then the system is in the orientational disordered phase. Whereas, when the system is in the ordered phase, the order parameter reaches to the maximum value $Q = 1$, namely all the individuals have the same orientation. On the other hand, the quantity ρ in Eq. (5) characterizes the spatial distribution of the individuals. Hence, the behavior of animals can be adequately described by the two parameters Q and ρ.

III. SIMULATION RESULTS

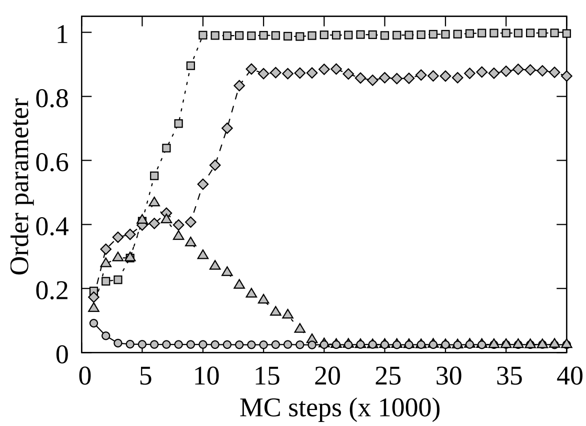

Fig. 1. The time dependence of order parameter with system size $N = 900$, $\xi = 0.05$, 0.25, 0.45 and 0.65 (circles, squares, diamonds and triangles, respectively)

We apply the algorithms of MC technique to the new model which have been described in Sec. II. For the model's parameters, we use $\varepsilon = 0.04$, $J = 1.0$ (taken as the unit of energy). The number of individuals are $N = 100$, 400 and 900 with the lattice size $L = 40, 80$ and 120, respectively. For testing the convergence of MC simulations, we show in figure 1 the time dependence of order parameter for a large system size $N = 900$ with $\xi = 0.05,\ 0.25,\ 0.45$ and 0.65. The order parameters are converged after 2×10^4 MC steps.

For the initial configuration, the positions on the lattice of all individuals and their orientations are randomly generated by an uniform distribution. At each Monte-Carlo step, we reset the internal state of all individuals to be excited state $S_i = 1$, then we randomly choose N_0 individuals (according to Eq. (2)), and set them to be non-excited state $S_i = 0$. Their position and orientation

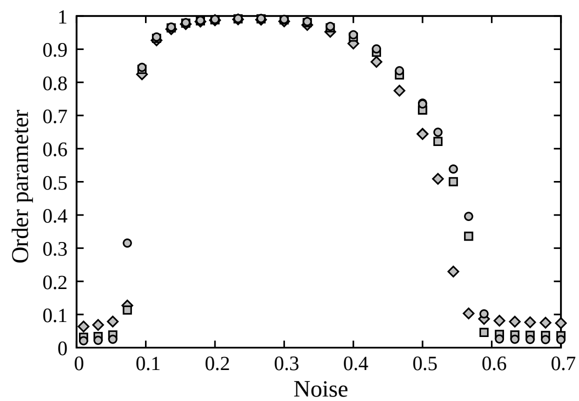

Fig. 2. Order parameter versus noise with the system sizes $N = 100$ (diamond), 400 (square) and 900 (circle)

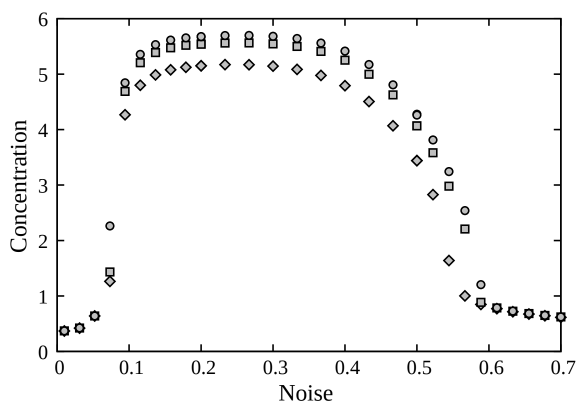

Fig. 3. Concentration versus noise with the system sizes $N = 100$ (diamonds), 400 (squares) and 900 (circles)

are updated by Metropolis algorithm. At each ξ, the equilibration time lies around 4×10^6 MC steps per individual and we compute statistical averages over 8×10^6 MC steps per individual. Periodic boundary conditions (PBCs) are used in the *xy* plane. We obtained the dependence of the order parameter and the concentration on the noise which are shown in the figures 2 and 3, respectively.

We see in Fig. 2 for $N = 100$, the system undergos two transitions at low noise $\xi^1 = 0.0768$ and high noise $\xi^2 = 0.541$. These transitions separate the system into three phases: phase I, II and III at low noise $\xi < 0.0768$, medium noise $0.0768 \leq \xi \leq 0.541$ and high noise $\xi > 0.541$, respectively. With increasing the system size, the transition noise ξ^2 increases from 0.541 to 0.584, while ξ^1 decreases from 0.0768 down to 0.0723.

In phase I, the order parameter $Q \simeq 0$, so the system is in the disordered phase. On the other hand, the concentration $\rho \simeq 0$ (see in Fig. 3), it indicates that the individuals are far away from each other. Therefore, this phase is equivalent to the uncollected behavior of animal group.

With increasing the noise, the order parameter Q increases up to 1.0 and the concentration ρ increases up to 5.9. The system undergos from disordered phase (phase I) to ordered phase (phase II) over the first transition ξ^1, then one slowly decreases in phase II until the noise reaches to the second transition ξ^2. In this phase, the individuals are close to each other with the same orientation. The ordered phase corresponds to the flocking behavior of animal group when they are faced with danger such as predators.

In the case of high noise, the system is changed from ordered phase (phase II) to melted phase (phase III) passing through the second transition. With increasing the noise, the order parameter and concentration rapidly decrease down to zero. Phase III is equivalent to the runaway behavior of animal group when they are under predator's attack. The difference between two phases (phase I and phase III) is that the particles in phase I are almost immobile while they are moving very fast in a disordered manner in phase III. Phase I is called free phase with a few contacts between the individuals because almost of them are non-excited, whereas all of them are excited in phase III.

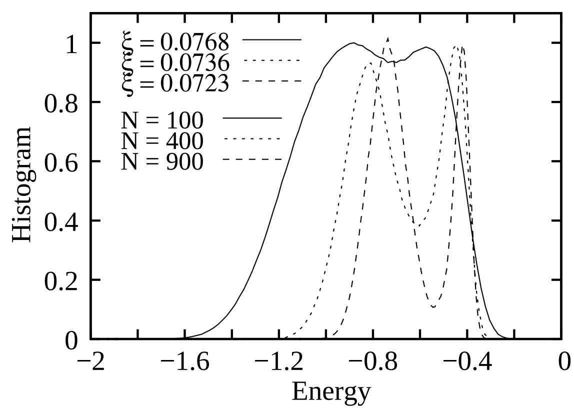

Fig. 4. Energy histogram versus energy at the first transition for three system sizes

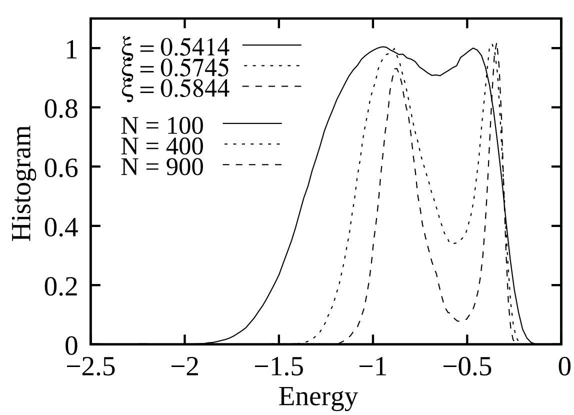

Fig. 5. Energy histogram versus energy at the second transition for three system sizes

Let us say a few words on the phase transition, the discontinuity in order parameter curve is a clear signature of a first-order transition. Of course, it is only one of the conditions for the first-order transition. To give a conclusion on that, we plot in figures 4 and 5 the energy histogram at two transitions I-II and II-III, for three system sizes $N = 100, 400$ and 900. The double-peak histograms are clearly shown for both transitions at low noise (Fig. 4) and high noise (Fig. 5). The dip between the two maxima becomes deeper with increasing size. Note that a “true” discontinuity happens only when the dip comes down to zero. The distance between the two peaks is then the latent heat. To see this, we need sizes much larger than $N = 900$. But this is out of the scope of our present purpose.

IV. CONCLUDING REMARKS

We have proposed in this paper a new model for studying the phase transition behavior of animal group. The group of animals is considered as a system of self-propelling particles with including an internal state. The external state of each individual has q states as in Potts model which is corresponding to q moving directions. The external state is similar to the definition of the individuals in the lattice gas model developed by Csahók *et al.* [18]. But in our model, the rules of interaction between the two individuals are controlled by their internal state, i.e., there is no interaction if and only if both individuals are in non-excited state. At a given external noise, there is only $N_e \leq N$ individuals are in excited state, while the remainder are in non-excited state.

The result presented here will serve as a testing for the new model. We showed that with increasing noise, the system has three phases I, II and III separated by two transitions, the first transition occurs at a low noise and and the second one at high noise. The three phases are disordered, ordered and melted phases which correspond respectively to the following behaviors of animals: uncollected state, flocking state and runaway state. Both transitions from one phase to another are found to be of the first-order. Note that the transition between disordered and ordered phases at low noise is unable for the observation using any previous models. Furthermore, the transition between uncollected to flocking states is an important behavior of the biological systems when they are faced with danger.

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