Lattice-gas model for collective biological motion

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A simple self-driven lattice-gas model for collective biological motion is introduced. We find a weakly-first-order phase transition from individual random walks to collective migration. A mean-field theory is presented to support the numerical results.

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I. INTRODUCTION

One of the most interesting aspects of evolution is the emergence of multicellular organisms due to the appearance of cooperation and differentiation of eukaryotes. Although much research has been done along this line, some of the related basic questions are still open. As a natural step towards the understanding of the physical and physicochemical background of self-organization of microorganisms several authors considered relatively simple systems such as the development of bacterial colonies.

The growth of bacterial colonies having complex geometries has been extensively studied recently [1–5]. One of the mean aspects was the fractality [6] of the growing colonies. It has been found that the framework of diffusion limited growth fits these phenomena well [1,3]. In addition, the various morphologies of growing colonies have been experimentally investigated recently [4] and a dynamical model has been introduced which incorporates a wide range of effects relevant to the phenomenon of collective bacterial growth and motion, for example, chemotaxis. In a further related model [7], aimed at describing the collective motion of self-driven particles (such as bacteria), a quasicontinuous approximation has been used with rules (particles moving with the same absolute velocity take on the average direction of motion of the neighboring particles) based on biological assumptions. As a main result it has been shown that spontaneous breaking of rotational symmetry can occur as the density of particles is increased or the level of random noise (i.e., the temperature) is lowered. The transition has been found to be continuous.

One of the basic differences between living and azoic systems is that living organisms are *self-driven*: they can transform energy gained from food into mechanical energy which allows them to change their position. As the simplest example we can take bacteria [8,9], having various ways of motion. One of the mechanisms is motion by the means of flagella: the bacteria have flagella functionally analogous to a propeller attached to a motor. The motion of organisms is not under control of an external field, as is common in physical systems. Instead, the environmental effects cause only a change in the local velocity of the organisms. Since living objects are capable of communicating in various ways (ranging from the sensing of chemicals to verbal communication among humans), an organism is in continuous interaction not only with its environment but also with other organisms in its neighborhood. Thus in the first approximation a system of organisms can be considered as an open interacting multiparticle physical system. Then one can attempt to apply the methods recently developed in the investigations of complex systems [10,11].

In this paper we present a simple lattice-gas model for the collective motion of self-driven particles. A similar approach has been applied to traffic systems [12–14] which also belong to the class of self-driven systems. Further approaches to self-driven systems include the reaction-diffusion description [15], investigation of the related integro-differential equations [16], molecular dynamics [17], and cellular automata [18,19].

The aim of this paper is to extend the usual statistical physical description for a particular case of collective motion in systems of living objects. First we introduce our model; then we give a theoretical description of the problem. In Sec. IV we present the numerical results and in Sec. V we summarize our results.

II. THE MODEL

Our model is defined on a triangular lattice of L^2 sites with unit lattice spacing and periodic boundary conditions. We put N particles (bacteria) on the lattice, where N is not necessarily smaller than the number of lattice sites. The density of the particles is defined as

$$\varrho = \frac{N}{L^2}. \tag{1}$$

Each site can be either empty or occupied by one or more particles. If more than one particle is present at a

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site then in the calculations only the lowest one will be considered, where the lowest particle is defined as having the smallest random number previously assigned to each particle.

The particles are characterized by their position $\mathbf{r}_i$ and velocity $\mathbf{v}_i$ $(i = 1, \ldots, N)$ which is of unit length $(|\mathbf{v}_i| = 1)$ and can point in any of the lattice directions ($\mathbf{u}_\alpha$, Fig. 1).

At one time step the positions and velocities of all particles are updated simultaneously according to the following rules.

(1) (a) For the particles which are not the lowest at their position we assign a random direction; (b) for the particles which are the lowest at their site we choose a new velocity $\mathbf{u}_\alpha$ from a Boltzmann distribution

$$P(\mathbf{u}_\alpha) = \frac{1}{\mathcal{Z}} \exp\left(-\beta \mathbf{u}_\alpha \sum_{j \in \mathrm{LNN}} \mathbf{v}_j\right),$$

where $\mathcal{Z}$ is a normalizing factor so that $\sum_{\alpha=1}^{6} P(\mathbf{u}_\alpha) = 1$, and β is $1/T$ $(k_B = 1)$. The summation goes over the nearest neighbors which are in the lowest position (LNN).

(2) Every particle is moved one lattice unit in the direction of its velocity:

$$\mathbf{r}_i \leftarrow \mathbf{r}_i + \mathbf{v}_i.$$

Note that the last step may result in sites with occupancy higher than 1; this is the reason why we have to deal with such cases. The motivation for step 1(a) is that we try to minimize the effect of multiple occupancy by letting the extra particles diffuse away. The temperature parameter is not connected to the ambient temperature of the bacterial colony, it is rather an effective value which depends on many external parameters, such as, for example, food concentration and agar humidity. The case of high food concentration is likely to be represented by high T values since then the bacteria can move faster and do not need coordinated behavior to extract food from the agar. On the other hand, when there is a food shortage the bacteria tend to cooperate, which results in a lower effective temperature. The above model is in its spirit close to the continuum model of self-driven particles [7]; however, the present version has a number of features which had to be introduced because of its discrete nature.

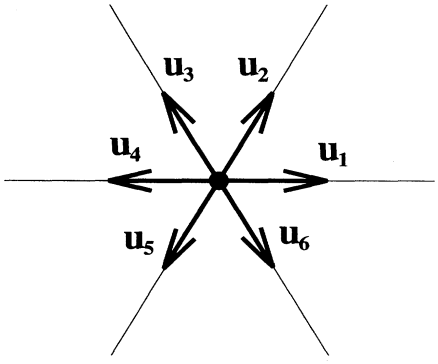

FIG. 1. One lattice site; the six lattice directions are shown.

One of the quantities of interest is the average velocity of the particles which we shall consider as the order parameter and define as

$$m = \frac{1}{N} \left| \sum_i \mathbf{v}_i \right|. \tag{2}$$

Obviously $0 \leq m \leq 1$ holds. To have a closer analogy with spin systems we define a Hamiltonian

$$H = -\frac{1}{2} \sum_{i,j \in \mathrm{LNN}} \mathbf{v}_i \cdot \mathbf{v}_j, \tag{3}$$

in accord with the simulation rule step 1. Those particles which are not the lowest at their position do not give a contribution to the energy; they are regarded as a free gas. The energy per particle is

$$\langle \varepsilon \rangle = \frac{E}{N}.$$

Having introduced the energy it is straightforward to define the heat capacity per particle,

$$c = \frac{\partial \varepsilon}{\partial T}.$$

Although we have similarities with spin systems our model differs in a very specific way: the spins in our model are *moving* and this spatial dynamics is coupled to the spin dynamics.

Figure 2 shows a possible time evolution of the position and velocities of five particles. The particles are lettered from A to E and the arrows show the direction of their velocity ($\mathbf{v}_i$). At time step (b) they form a cluster (containing a doubly occupied site) which then gradually breaks up.

III. THEORY

Our system is closely related to the six-state Potts model [20] since we have $q = 6$ possible velocity states for a particle. Unlike the Potts model these states are not orthogonal, and we have an essentially nonequilibrium system; nevertheless, a mean-field theory can be constructed in a similar way [21].

First we introduce a mean-field Hamiltonian instead of Eq. (3):

$$H_{\mathrm{MF}} = -\frac{1}{2} \sum_{i,j \in \mathrm{L}} \mathbf{v}_i \cdot \mathbf{v}_j, \tag{4}$$

where the summation goes over all *lowest* (L) particles, not only the nearest neighbors. The mean-field energy function can be written as

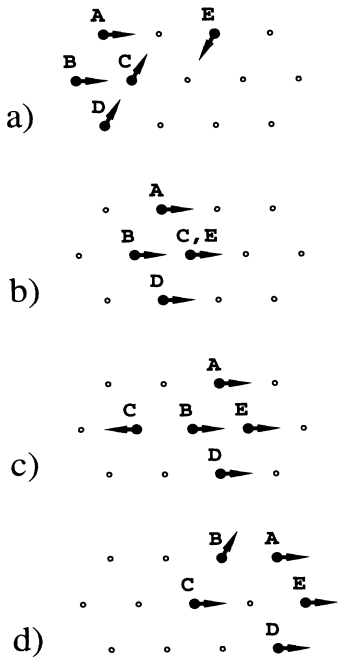

FIG. 2. A possible time evolution of our model (a)→ (d) shown on a small portion of the lattice. Note the double occupancy in time step (b).

$$E_{\mathrm{MF}} = -\frac{1}{2} N \varrho_{\mathrm{eff}} \sum_{\alpha,\gamma=1}^{6} x_\alpha U_{\alpha\gamma} x_\gamma, \tag{5}$$

where $\varrho_{\mathrm{eff}} = 1 - \exp(-\varrho)$ is the effective density, i.e., a site has on average $6\varrho_{\mathrm{eff}}$ occupied neighboring sites, x_α is the fraction of particles traveling in the lattice direction α ($\sum_{\alpha=1}^{6} x_\alpha = 1$), and $U_{\alpha\gamma} = \mathbf{u}_\alpha \cdot \mathbf{u}_\gamma$ which for the case of the Potts model would be simply $U_{\alpha\gamma} = \delta_{\alpha\gamma}$.

The average energy per particle is

$$\varepsilon_{\mathrm{MF}} = \frac{E_{\mathrm{MF}}}{N} = -\frac{1}{2} \varrho_{\mathrm{eff}} \sum_{\alpha,\gamma=1}^{6} x_\alpha U_{\alpha\gamma} x_\gamma. \tag{6}$$

The entropy per particle is

$$s_{\mathrm{MF}} = -\sum_{\alpha=1}^{6} x_\alpha \ln x_\alpha,$$

so for the free energy per particle one gets

$$\beta f_{\mathrm{MF}} = \beta \frac{F_{\mathrm{MF}}}{N} = \sum_{\alpha=1}^{6} \left(x_\alpha \ln x_\alpha - \frac{1}{2} \varrho_{\mathrm{eff}} \beta x_\alpha \sum_{\gamma=1}^{6} U_{\alpha\gamma} x_\gamma \right). \tag{7}$$

We intend to find the configuration x_α which minimizes the free energy f_{MF}. Since all the lattice directions are equivalent we can look for a solution in the form of

$$x_1 = \frac{1}{6} + \frac{5}{6} m_{\mathrm{MF}} \tag{8}$$

and

$$x_{\alpha>1} = \frac{1}{6} - \frac{m_{\mathrm{MF}}}{6}, \tag{9}$$

where m_{MF} is the mean-field order parameter which satisfies the relation

$$m_{\mathrm{MF}} = \left| \sum_{\alpha=1}^{6} x_\alpha \mathbf{u}_\alpha \right|$$

according to Eq. (2). Substituting Eq. (8) and Eq. (9) into Eq. (7) after some algebra one gets for the mean-field free energy

$$\beta f_{\mathrm{MF}} = -\frac{1}{2} \varrho_{\mathrm{eff}} \beta\, m_{\mathrm{MF}}^2 - \ln \frac{1}{6} + \frac{5(1 - m_{\mathrm{MF}})}{6} \ln \frac{1 - m_{\mathrm{MF}}}{6} + \frac{1 + 5m_{\mathrm{MF}}}{6} \ln \frac{1 + 5m_{\mathrm{MF}}}{6}. \tag{10}$$

For high temperatures ($T > T_c$) this function has its minimum at $m_{\mathrm{MF}} = 0$ which corresponds to the disordered state of the system. At the critical temperature, which can be derived from f_{MF} and in our case is

$$T_c \approx \frac{\varrho_{\mathrm{eff}}}{3.353}, \tag{11}$$

a nontrivial minimum appears. The phase transition, as in the six-state Potts model [22], is first order. The jump in the order parameter in this approximation is given exactly by

$$\Delta m_{\mathrm{MF}} = 0.8.$$

IV. NUMERICAL RESULTS

We have studied our systems by Monte Carlo simulations. For the initial configuration we chose a random distribution for the position and velocity of the particles. Typical configurations of the system for various temperatures T and particle densities ϱ are shown in Fig. 3. It can be easily seen that at low temperature the particles tend to form clusters as can be expected.

We have performed several long-time runs to obtain the behavior of the quantities defined in Sec. II as a function of T and ϱ. We used various system sizes (L) up to 40 for high densities and up to 200 for low densities. The limiting factor was the convergence time which for the case of our largest system was on the order of 10^6 sweeps of the system. Figure 4 demonstrates the order parameter as a function of the temperature for $\varrho = 0.9$. The estimated jump at T_c is smaller but close to the value obtained by the mean-field theory. In Fig. 5 we present the average energy which is also subject to a finite jump at T_c. These two figures suggest that a first-order phase transition takes place at $T = T_c$ in agreement with the theoretical prediction. Strong evidence supporting this idea is presented in Fig. 6, where we have plotted the dis-

tribution $P(\varepsilon)$ of the energy values for a number of different temperatures below and above T_c. One can clearly see a gap in the distributions at intermediate energies which is a unique feature of first-order phase transitions [23]. The inset in the figure shows the distribution for an Ising type interaction of nonmoving particles in the same system where the transition is known to be second order. In Fig. 7 we present the temperature dependence of the heat capacity which is the measure of the broadness of the energy distribution. A characteristic peak can be observed near T_c. The position of the peak is shifted for various lattice sizes due to finite size effects.

We studied the behavior of the model also as a function of density of particles (ϱ). Figure 8 shows the temperature dependence of the average energy for various densities obtained. The transition is present even for very small densities although the position of the critical temperature is lowered. In Fig. 9, we have plotted the dependence of the transition temperature on the density. There is a natural distinction between the high and low density regimes of the system: at the percolation threshold the behavior of the system is expected to change. In fact we observe a change in the dependency of the critical temperature below the percolation threshold of the

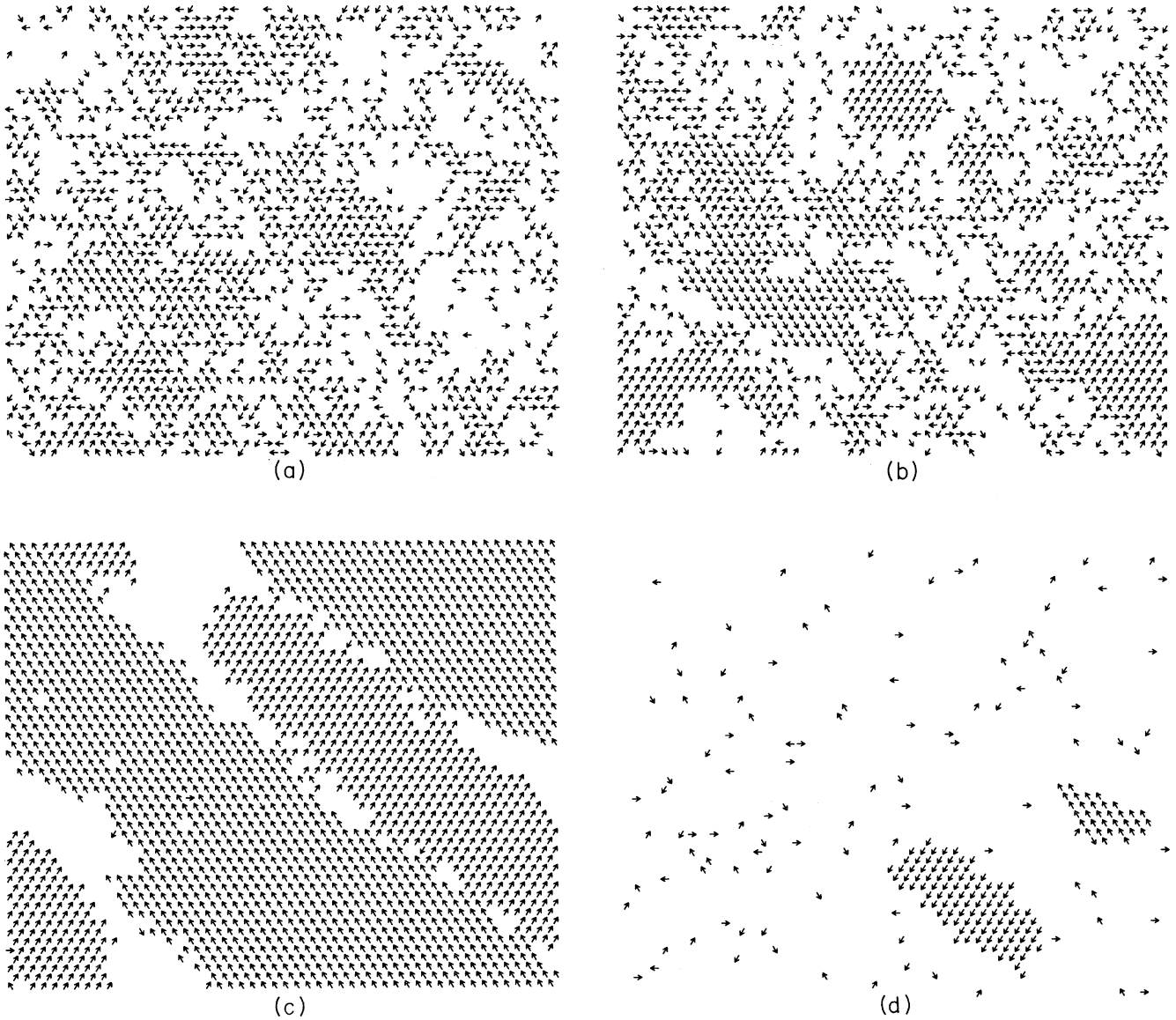

FIG. 3. Some typical snapshots of the system at (a) high temperature, (b) intermediate temperature, (c) low temperature at $\varrho = 0.9$, and (d) intermediate temperature at a lower density. Note the appearance of ordered clusters. (Only the particles in lowest position are drawn.)

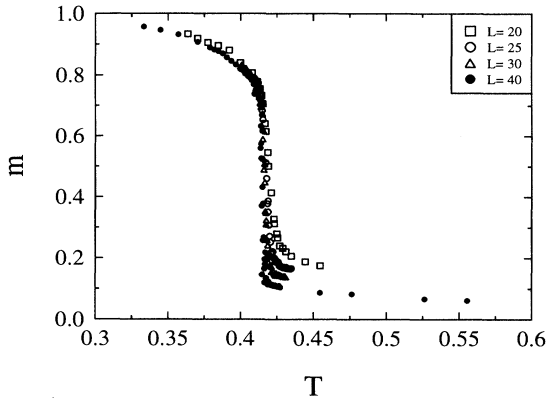

FIG. 4. The order parameter (m) as a function of the temperature (T) for density $\varrho = 0.9$.

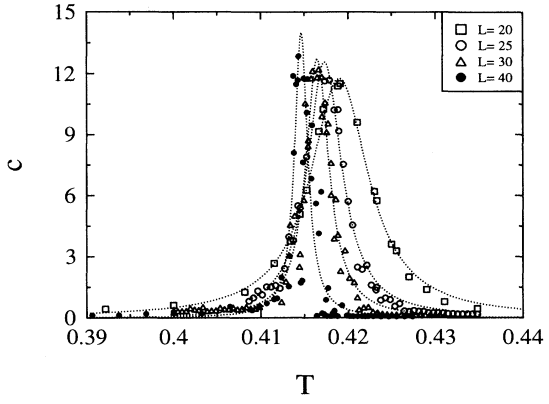

FIG. 7. The heat capacity (c) versus temperature graph for the systems as on Fig. 4. The dotted lines are guides to the eye.

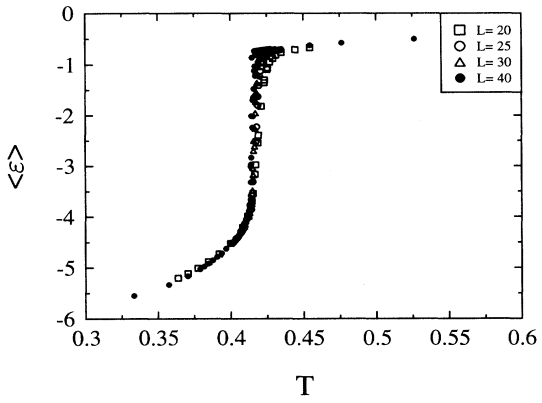

FIG. 5. The average energy ($\langle\varepsilon\rangle$) versus the temperature in the same systems as on Fig. 4.

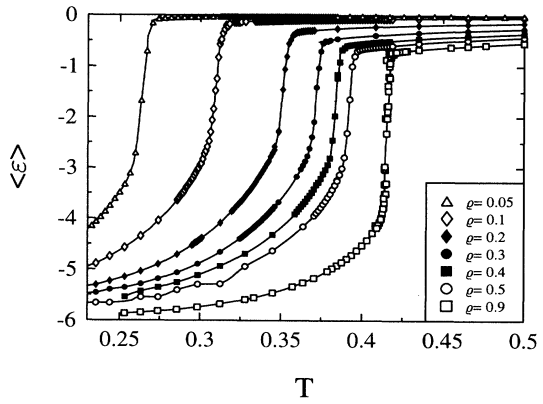

FIG. 8. The average energy as a function of temperature for various densities of particles.

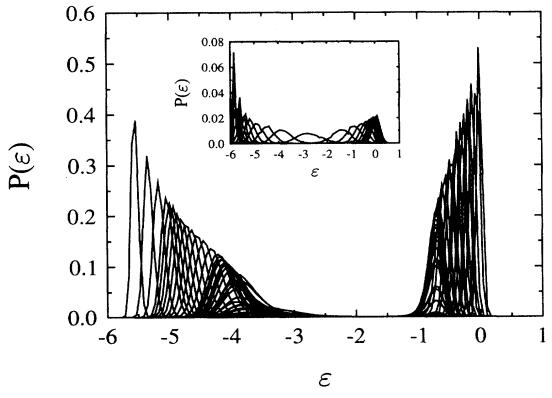

FIG. 6. The energy distribution [$P(\varepsilon)$] for various temperatures below and above the transition ($\varrho = 0.9$). Note the energy gap between $\varepsilon \approx -1$ and $\varepsilon \approx -3.5$. Inset shows the distribution for Ising spins instead of mobile particles where the transition is continuous.

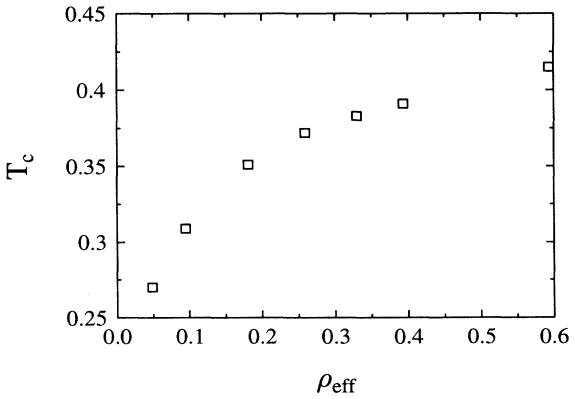

FIG. 9. The critical temperature as a function of the density of particles.

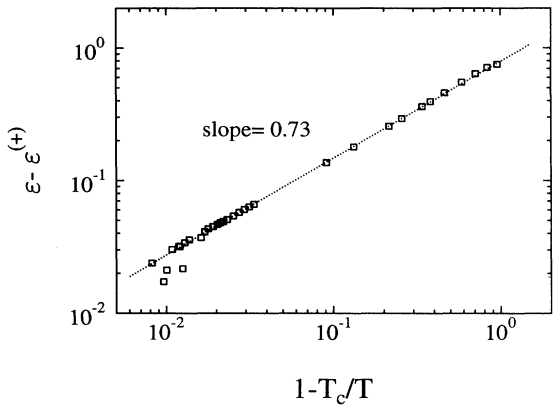

FIG. 10. Energy difference versus temperature for $\varrho = 0.9$. ($T_c = 0.413, \varepsilon^{(+)} = -0.76$.)

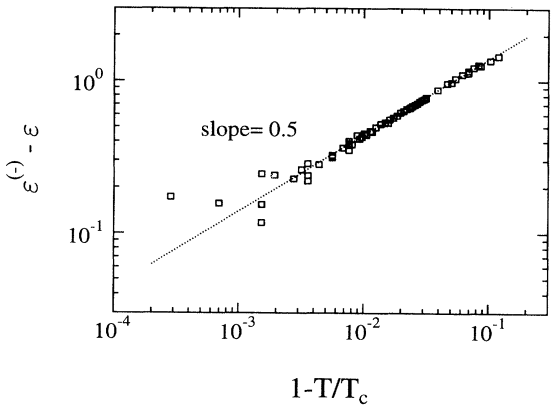

FIG. 11. Energy difference versus temperature for $\varrho = 0.9$. ($T_c = 0.413, \varepsilon^{(-)} = -3.75$.)

triangular lattice ($\varrho = 1/2$ and $\varrho_{\text{eff}} \approx 0.39$) at $\varrho_{\text{eff}} \approx 0.25$ which corresponds to density $\varrho \approx 0.29$. The values of the measured critical temperatures are higher than the one obtained from Eq. (11) which shows the boundaries of applicability of our mean-field approximation.

The behavior of the average energy of the Potts model near its transition temperature can be characterized by two exponents $\alpha^{(-)}$ and $\alpha^{(+)}$ [22]. These exponents are present due to the weakly-first-order nature of the transition. The temperature dependence of the average energy is given by

$$\langle \varepsilon \rangle = \varepsilon^{(-)} - A^{(-)}(1 - T/T_c)^{1-\alpha^{(-)}} \tag{12}$$

for $T < T_c$ and similarly

$$\langle \varepsilon \rangle = \varepsilon^{(+)} + A^{(+)}(1 - T_c/T)^{1-\alpha^{(+)}} \tag{13}$$

for $T > T_c$. The difference between $\varepsilon^{(+)}$ and $\varepsilon^{(-)}$ is equal to the energy jump during the phase transition. In Fig. 10 and Fig. 11 we plotted the energy differences versus the temperature according to Eq. (12) and Eq. (13) for $\varrho = 0.9$. The exponents obtained from the slopes are

$$\alpha^{(+)} \approx 1 - 0.73 = 0.27$$

and

$$\alpha^{(-)} \approx 1 - 0.5 = 0.5.$$

These values are different both from those of the $q = 6$ state Potts model ($\alpha^{(+)} \approx 0.7$ and $\alpha^{(-)} \approx 0.7$) and in part from the corresponding mean-field values ($\alpha^{(+)} = \alpha^{(-)} = 1/2$).

V. CONCLUSION

We have presented a lattice-gas model for collective biological motion. We have shown both numerically and theoretically that a weakly-first-order phase transition takes place in our system separating the phase with zero net transport and the ordered phase with nonzero average velocity. We find the exponents $\alpha^{(+)}$ and $\alpha^{(-)}$ differ from the ones of the $q = 6$ Potts model and from mean-field values. This difference can be attributed to the fact that although we have similarities with spin systems our model differs in a very specific way: the spins in our model are *moving* and this spatial dynamics is coupled to the spin dynamics. It is remarkable that the behavior of the present lattice model is qualitatively different from that of the analogous continuum model [7]. While in the continuum model and in a directly related continuum equation for a two-dimensional dynamic XY model [24] a second-order transition was observed, in our lattice-gas version the transition is more complex and has a first-order component. Such discrepancies, however, are not unfamiliar even in two-dimensional equilibrium systems: in particular, there is no long range ordering in the equilibrium XY model [25] having continuous symmetry, while its discrete counterparts (i.e., the Ising model) exhibit a second-order phase transition.

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