Lattice Boltzmann simulation for the energy and entropy of excitable systems*

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(Received 1 March 2010; revised manuscript received 21 October 2010)

The internal energy and the spatiotemporal entropy of excitable systems are investigated with the lattice Boltzmann method. The numerical results show that the breakup of spiral wave is attributed to the inadequate supply of energy, i.e., the internal energy of system is smaller than the energy of self-sustained spiral wave. It is observed that the average internal energy of a regular wave state reduces with its spatiotemporal entropy decreasing. Interestingly, although the energy difference between two regular wave states is very small, the different states can be distinguished obviously due to the large difference between their spatiotemporal entropies. In addition, when the unstable spiral wave converts into the spatiotemporal chaos, the internal energy of system decreases, while the spatiotemporal entropy increases, which behaves as the thermodynamic entropy in an isolated system.

Keywords: lattice Boltzmann method, energy, entropy, spiral wave

PACS: 05.50.+q, 05.10.–a, 05.45.–a **DOI:** 10.1088/1674-1056/20/2/020510

1. Introduction

The medical research indicates that the cardiac tissue belongs to an excitable medium. If the spiral waves occur in cardiac tissue, it causes ventricular tachycardia. However, when the spiral wave breaks up into spatiotemporal chaos through Doppler effects, the electrocardiogram shows ventricular fibrillation.[1−3] It is quite attractive to consider the quantitative description of the spatiotemporal pattern occurring in cardiac tissue. The information about the cardiac behaviour, which can be applied to the prevention and the cure of heart disease, is thus obtained when relevant variables are measured. Different formulas of entropy have been developed to characterize spatiotemporal behaviours.[4,5] In the present paper we develop the measure of spatiotemporal behaviour in an excitable system. We focus our attention on the energy and the entropy of an excitable system because the dissipative structure needs energy to be maintained and the order degree of system can be described through the entropy.

Lattice Boltzmann method (LBM) is a powerful approach, which was simplified by Qian *et al.*[6] and Chen *et al.*[7] for proposing the single-relaxation collision term at the beginning of the 90's last century. The LBM has been widely used in different systems, such as fluid,[8,9] traffic flow,[10] thermodynamic system,[11 and reaction diffusion system.[12] In this method, the space and the time are discrete while the state of the system is continuous. The differential equation which describes the evolution of the complex system can be obtained from the evolution equation of LBM, so the macroscopical rule of the complex system can be studied by using the LBM. An important advantage of the LBM is that the microcosmic physical interactions of the particles can be conveniently incorporated into the numerical model, thus it bridges the gap between the microscopic world and the macroscopic phenomenon, and can conveniently to determine the entropy and the internal energy of the system. Using the LBM, we have studied the production and the evolution of spiral wave in the excitable Selkov system,[13] the relation between wavelength and wave speed,[14] and the particle velocity distribution.[15] In the present paper, we study the internal energy and the spatiotemporal entropy of the system. By determining the internal energy and the spatiotemporal entropy correctly, we find that these variables can describe the state of the system very well. The spatiotemporal entropy indicates clearly the transition from spiral wave to spatiotemporal chaos, as well as the difference between different types of waves. The physical mechanism behind the breakup of spiral

*Project supported by the National Natural Science Foundation of China (Grant Nos. 10765002, 10562001 and 81060307).
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wave is obtained.

The remainder of the present paper is organized as follows. In Section 2 we introduce the Selkov reaction–diffusion system and the LBM simply. In Section 3 the internal energy and the spatiotemporal entropy of the system are introduced. The numerical results and their discussion are given. The conclusions are drawn in Section 4 finally.

2. Selkov model and LBM

2.1. Selkov model

The Selkov reaction–diffusion model was originally constructed to describe certain aspects of glycolysis. The dimensionless dynamics equations take the form as[16]

$$\frac{\partial \rho_1}{\partial t} = (\alpha - \chi\rho_1 - \rho_1\rho_2^2 + \kappa\rho_2^3) + D_1\nabla^2\rho_1, \quad (1a)$$

$$\frac{\partial \rho_2}{\partial t} = (\beta - \rho_2 + \rho_1\rho_2^2 - \kappa\rho_2^3) + D_2\nabla^2\rho_2, \quad (1b)$$

where the variables ρ_1 and ρ_2 represent the concentrations of the species 1 and 2, respectively; D_1 and D_2 are the diffusion coefficients; α, β, χ, and κ are system parameters. The Selkov system described by Eq. (1) is an excitable system with the correct parameters.[17]

2.2. LBM

A particular two-dimensional LBE model considered in this work is the 5-velocity model (2DQ5 model).[13] In this model, space is discretized into square lattices. There are five discrete velocities described by $\boldsymbol{e}_k$, where the k represents the direction of the velocity: $k = 0$ shows the rest state, $k = 1,\ 2,\ 3,\ 4$ denote right, up, left, and down directions, respectively. The above discrete velocities correspond to the particle motion from a lattice node $\boldsymbol{r}$ to one of the 4 nearest neighbours. The distribution function $f_s(\boldsymbol{r}, \boldsymbol{e}_k, t) = f_{sk}$ describes the probability of the species s ($s = 1, 2$) with the velocity $\boldsymbol{e}_k$ on site $\boldsymbol{r}$ and at time t. The equilibrium distribution function is written as $f_s^{\rm eq}(\boldsymbol{r}, \boldsymbol{e}_k, t)$. The concentration $\rho_s(\boldsymbol{r}, t)$ can be evaluated by

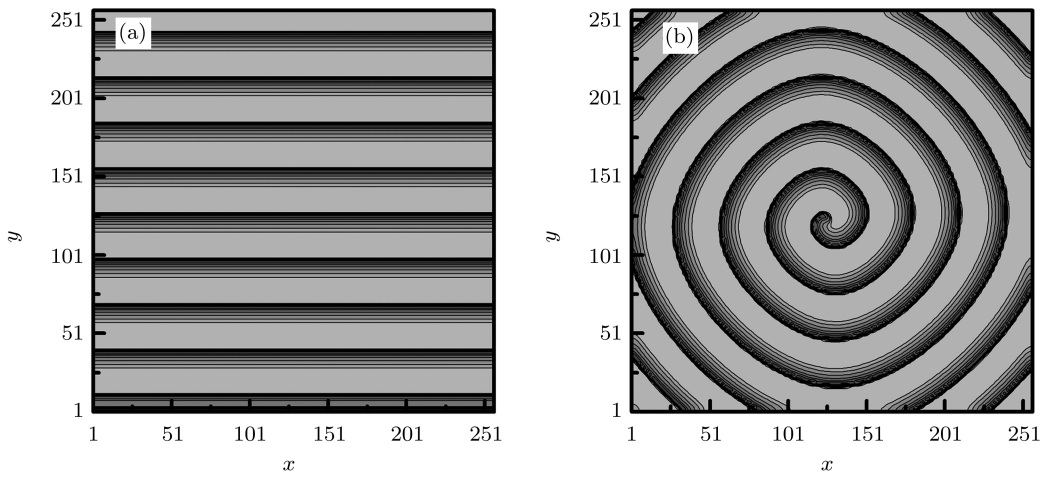
$$\rho_s(r, t) = \sum_{k=0}^{4} f_s(\boldsymbol{r}, \boldsymbol{e}_k, t). \quad (2)$$

The evolution equation of the f_{sk} is

$$f_s(\boldsymbol{r} + \boldsymbol{e}_k, \boldsymbol{e}_k, t+1) - f_s(\boldsymbol{r}, \boldsymbol{e}_k, t) = -\frac{1}{\tau_s}[f_s(\boldsymbol{r}, \boldsymbol{e}_k, t) - f_s^{\rm eq}(\boldsymbol{r}, \boldsymbol{e}_k, t)] + R_{sk}(\boldsymbol{r}, t), \quad (3)$$

where $R_{sk}(\boldsymbol{r}, t)$ denotes the change of ρ_s in direction k due to the reaction and τ_s is the relaxation time of species s. Using the multi-scale method and the Taylor-expand method, we can obtain Eq. (1) through Eq. (3),[13] so we can obtain the solution of Eq. (1) by solving Eq. (3) numerically.

According to the above LBM, the computer simulation is conducted for Selkov system with $\alpha = 0.77064$, $\beta = 0.0208$, $\chi = 0.1$, and $\kappa = 5.0$. The Selkov system is excitable when those parameters are applied. Throughout the paper, initial concentrations $\rho_1 = 7.65978$ and $\rho_2 = 0.02582$, which are the equilibrium values of ρ_1 and ρ_2, are applied. No-flux boundary conditions are used in all simulations. The spatial discretization of a 256×256 grid is performed. If the concentrations ρ_1 and ρ_2 at the lower boundary of the system are fixed at $\rho_1 = 6.5$ and $\rho_2 = 0.8$, the stable plane wave will be produced (see Fig. 1(a)). A



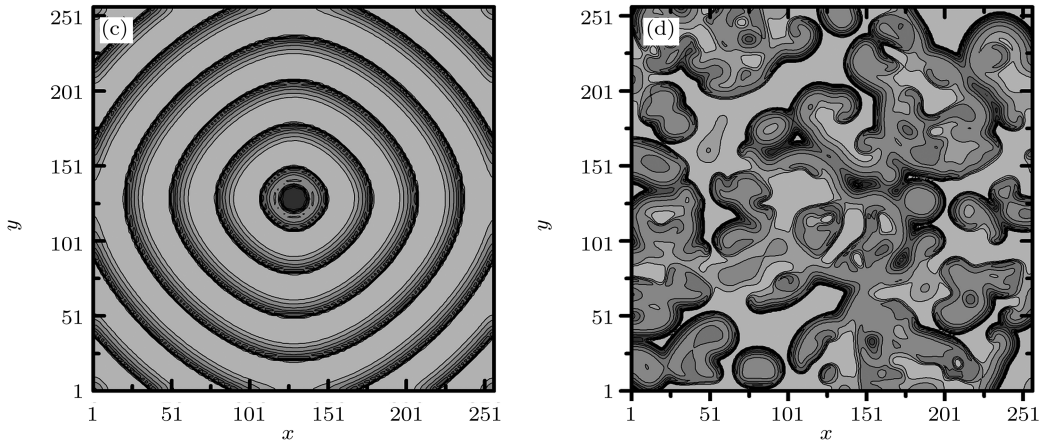


Fig. 1. Spatiotemporal patters of the Selkov model: (a) plane wave; (b) spiral wave; (c) target wave; and (d) spatiotemporal chaos.

spiral wave can be generated by truncating the plane wave and then removing one of two sections of the wave train (see Fig. 1(b)). When the concentrations ρ_1 and ρ_2 inside the disk-like region with radius $R = 8$ in the centre of the medium are fixed at $\rho_1 = 6.5$ and $\rho_2 = 0.8$, a target wave can be generated (see Fig. 1(c)). If the value of the parameter α is modified to be 0.75 while the other parameters keep unchanged, the spiral wave will be unstable and the spiral wave will break up into spatiotemporal chaos after some transient rotations, see Fig. 1(d). In the next section, we will discuss the internal energy and the spatiotemporal entropy of the above state of the system.

3. Internal energy and spatiotemporal entropy

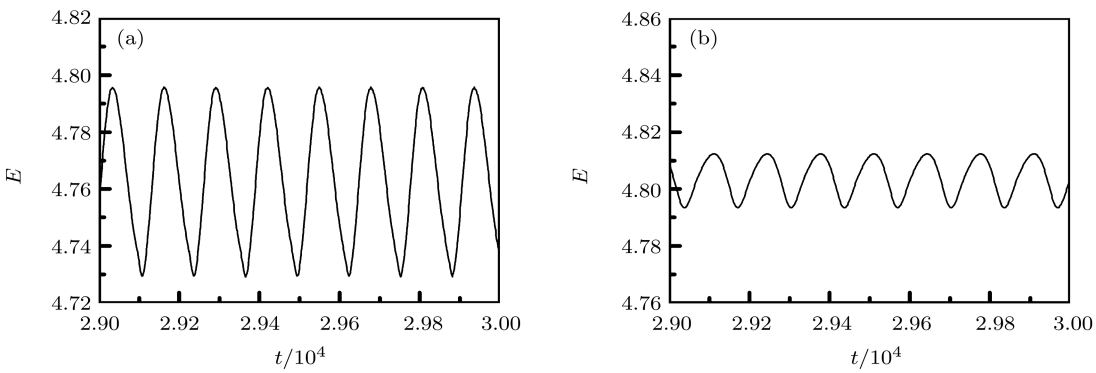
3.1. Internal energy

It is well known that the total energy of all the particles moving randomly is the internal energy of the system. According to the theory of LBM,[18] the internal energy of the system can be defined as

$$E = \frac{1}{N_x \times N_y}\left[\sum_{i=1}^{256}\sum_{j=1}^{256}\sum_{k=0}^{4}\frac{1}{2}e_k^2 f_1(i,j,k) + \sum_{i=1}^{256}\sum_{j=1}^{256}\sum_{k=0}^{4}\frac{1}{2}e_k^2 f_2(i,j,k)\right], \quad (4)$$

where i and j represent the grid indices. For the spatial discretization of a 256×256 grid, the values of N_x and N_y are both 256.

It is generally accepted that the maintenance of the dissipation-construction such as the spiral wave needs the sustaining of the internal energy, and the states of different systems have different internal energies. As long as the internal energy of a system is smaller than the energy of sustaining the dissipation-construction, the spatiotemporal-construction will be destroyed. Do the different states of a system have the same energy? How much energy do the different dissipation-constructions need? Nobody has discussed these problems so far. Therefore, we calculate the energies of the states as shown in Fig. 1. The results are shown in Fig. 2. After simple calculation,



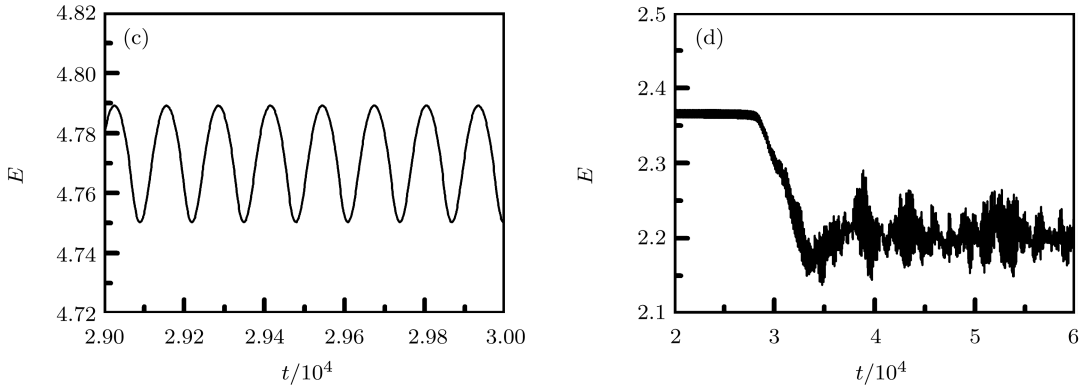


Fig. 2. Evolutions of energy E for (a) stable plane wave, (b) stable spiral wave, (c) stable target wave, (d) unstable spiral wave.

we can find from Figs. 2(a)–2(c) that the average energies of plane wave, target wave, and spiral wave are 4.76405, 4.77176 and 4.80410, respectively, which implies that under the same system parameters, the difference in average energy between different states is very small. Therefore, we can conclude that the same systems have the same average internal energy for different states. A comparison among Figs. 2(a)–2(c) and Fig. 2(d) clearly shows that the systems with different parameters have different internal energies. Especially, the conclusion drawn from the comparison between Fig. 2(b) and Fig. 2(d) is that the internal energy of spatiotemporal chaos state is much smaller than that of spiral wave, which means that the instability of the spiral wave is caused by the inadequate supply of energy.

3.2. Spatiotemporal entropy

The order degree of a system can be measured by the entropy. The concept of entropy can be expressed in terms of probability of various particle clusters based on Shannon entropy.[19,20] We call the entropy the spatiotemporal entropy because it reflects the complexity of the spatiotemporal pattern.

3.2.1. Particle velocity distribution

Now we focus our attention on the distribution of particle velocities in the spiral wave breakup process. The velocity of a particle on site $\boldsymbol{r}$ and at the moment t is given by the maximal distribution function. For example, if the maximal distribution function on site $\boldsymbol{r}$ and at time t is $f_s(\boldsymbol{r}, \boldsymbol{e}_3, t)$, then the velocity of the corresponding particle is $\boldsymbol{e}_3$. If the distribution function gives the same probability to different velocities, then we may randomly select one of them as the velocity of the particle. The computer simulation results are shown in Fig. 3. In order to obtain a clear image, only the velocity distribution of the particle around the spiral tip is shown here.

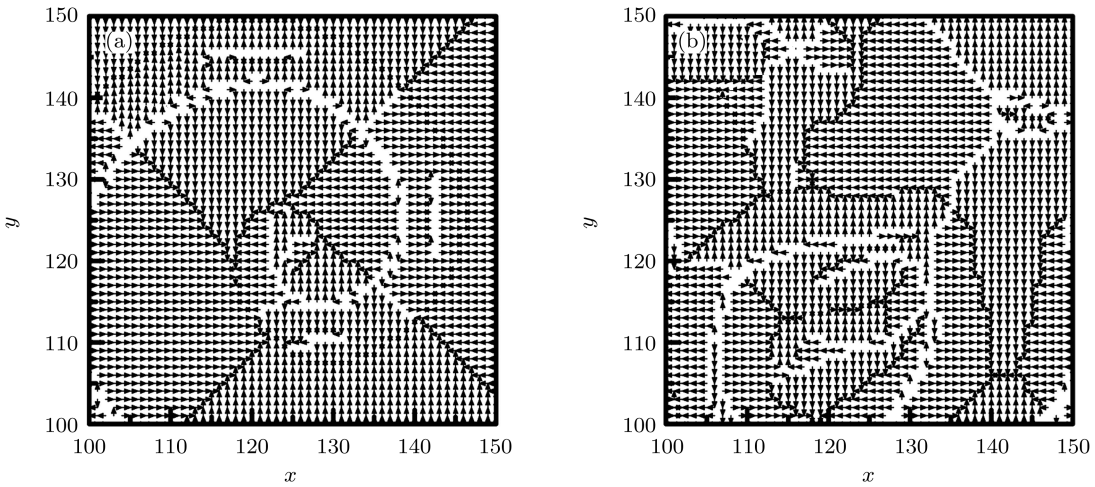


Fig. 3. Images of velocity field for (a) spiral wave, (b) spatiotemporal chaos, with parameters being the same as those in Fig. 1(d).

From Fig. 3, one can observe that the velocity field of spiral wave state can be divided into some particle clusters. The particles in a cluster have the same velocity, and the boundaries of the clusters are clear and continuous. The boundary lines of the clusters are spiral. When the system falls into spatiotemporal chaos, the original boundaries of the clusters are destroyed. The system has more particle clusters, and so the order degree of the system decreases.

3.2.2. Spatiotemporal entropy

Since the velocity fields of spiral wave and spatiotemporal chaos are different, we can define the spatiotemporal entropy as follows. Suppose that the number of particles in a cluster is M_i, and then the probability of the cluster can be defined as $p_i = M_i/(N_x \times N_y)$, where $N_x = N_y = 256$. According to the Shannon entropy,[19,20] the spatiotemporal entropy can be defined as

$$S = -\sum_{i=1}^{m} p_i \ln p_i, \tag{5}$$

where m is the number of the clusters. According to Eq. (5), the computer simulations are conducted separately for the plane wave, the target wave, and the spiral wave with the same parameters as those in Fig. 1. The results are shown in Fig. 4(a). We can find that the spatiotemporal entropy of target wave is bigger than that of plane wave, but the spatiotemporal entropy of spiral wave is biggest among those of the three waves. It is generally accepted that the smaller the spatiotemporal entropy, the more orderly the spatiotemporal pattern is. Comparing Fig. 4(a) with Figs. 2(a)–2(c), we can conclude that under the same system parameters, the higher the order degree of system, the smaller the average internal energy of the system is, which means that the state with higher order degree needs smaller average energy. On the other hand, the computer simulation result of spatiotemporal entropy for the instable spiral wave is shown in Fig. 4(b). The figure 4(b) shows that the spatiotemporal entropy of unstable spiral wave is higher than that of the initial spiral wave. Combining Fig. 4(b) with Fig. 2(d) leads to the conclusion that when a spiral wave state is destabilized, the system always evolves into the other state which has a higher spatiotemporal entropy and a lower internal energy. The above results enrich the knowledge about the entropy and the energy of the extended system.

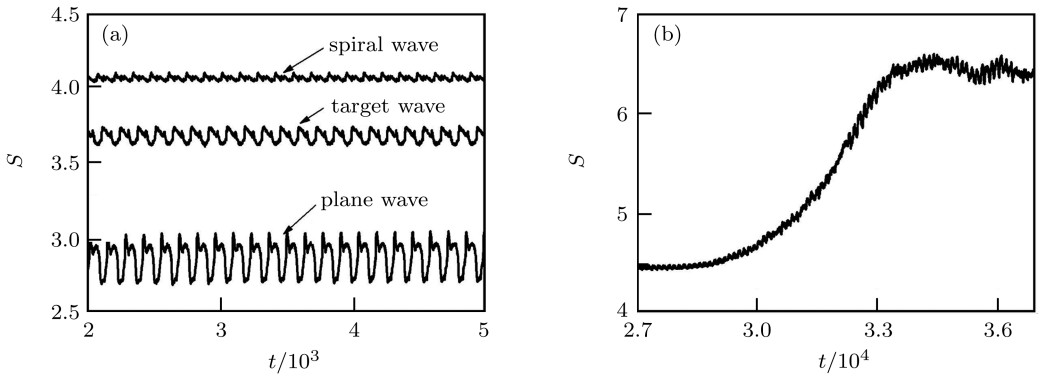


Fig. 4. Evolutions of entropy S for (a) different stable states and (b) spiral wave breakup.

4. Conclusions

We studied the internal energy and the spatiotemporal entropy by using the LBM. With abundant simulations of different states, we found that spiral wave loses its stability when the energy of the system is smaller than that of a stable spiral wave. In addition, the smaller the spatiotemporal entropy of the stable wave state in the same system, the less average energy the system needs. The spatiotemporal entropy increases when the transition from the unstable spiral wave to the spatiotemporal chaos occurs, which behaves as the thermodynamic entropy in an isolated system.

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