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WAVES AND THEIR INTERACTIONS IN THE LATTICE LOTKA-VOLTERRA MODEL

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In this work, we study the Lattice Lotka-Volterra model and specifically the properties of the waves that arise from inhomogeneous initial conditions. We consider different types of waves (stripe-like, radial, spirals) and we study their collision rules.

Introduction

The reactive dynamics of systems restricted to low dimensional supports are known to produce very rich and complex spatiotemporal behavior [1-8]. In particular, reactions that take place on a catalytic surface are a special category of reactive systems, that due to their low diffusivity and special spatial features, tend to produce interesting dynamical behavior. Examples of this kind of reactions are the CO oxidation on Pt surface [9-11], the NO reduction on Pt surface [11-14] and the NO+CO reaction on Pt [15,16].

To understand and describe the complex behavior of such reactions as well as analyze the underlying dynamical mechanisms, it is common to employ simplified reactive models, such as the Lattice Lotka-Volterra (LLV) model [2,8]. The LLV-model is a cyclic bimolecular model which involves three species X_1, X_2 and S. It has been studied in the literature as an alternative model to the usual Lotka-Volterra [17,18] since it also presents conservative Mean-Field (MF) dynamics (see e.g. [19,20]). The LLV-model is described by the following reaction scheme:

$$X_1 + X_2 \xrightarrow{k_2} 2X_2, \tag{1a}$$

$$X_2 + S \xrightarrow{k_1} 2S, \tag{1b}$$

$$S + X_1 \xrightarrow{k_2} 2X_1. \tag{1c}$$

In these reactions X_1 and X_2 correspond to two adsorbed chemical species while S denotes the empty sites of the catalyst. In that sense, we have an open reactive system, where reaction (1a) is an autocatalytic reactive step, (1b) denotes cooperative desorption while (1c) cooperative adsorption. The key ingredient of chemical nonlinearity is the

autocatalytic nature of the above reaction scheme. The homogeneous MF equations corresponding to the above scheme are:

$$dx_1/dt = k_2 x_1 s - k_s x_1 x_2, \tag{2a}$$

$$dx_2/dt = k_s x_2 x_1 - k_1 x_2 s, \tag{2b}$$

$$ds/dt = k_1 x_2 s - k_2 x_1 s. \tag{2c}$$

Here x_1 is the concentration of particles X_1, x_2 is the concentration of X_2 while s is the concentration of empty sites. From conservation of the total number of lattice sites we have thus:

$$x_1 + x_2 + s = 1. \tag{3}$$

To reduce the number of parameters we perform the following rescaling [8]:

$$a_1 = k_1/(k_1+k_2+k_s), \tag{4a}$$

$$a_2 = k_2/(k_1+k_2+k_s), \tag{4b}$$

$$\tau = t\,(k_1+k_2+k_s). \tag{4c}$$

Using Eqs (4) and (3), eqs (2) are transformed into a reduced and dimensionless form, namely:

$$dx_1/d\tau = a_2 x_1[1-x_1-x_2(1-a_1)/a_2], \tag{5a}$$

$$dx_2/d\tau = -a_1 x_2[1-x_1(1-a_2)/a_1-x_2]. \tag{5b}$$

Eqs (5) have four fixed points. Three of them, (0,0), (1,0), (0,1) are saddles and one of them (a_1,a_2) is a center surrounded by an infinity of closed periodic orbits [8,9]. The phase-space portrait can be seen in Fig. 1. We also give a characteristic MF temporal evolution in Fig. 2.

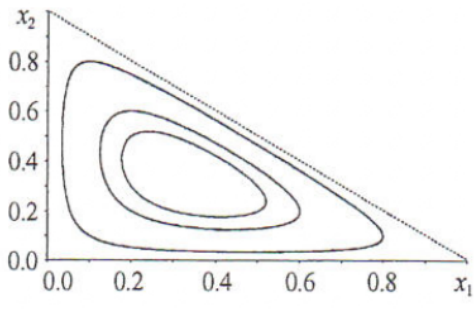

Fig. 1. Phase-space for a_1=0.333, a_2=0.333

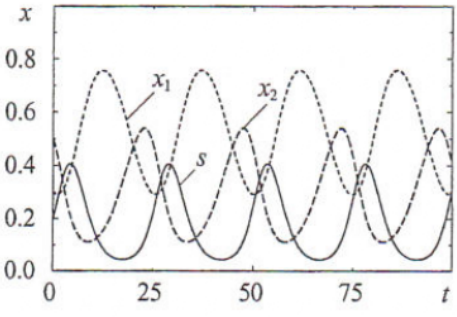

Fig. 2. Time evolution for a_1=0.53, a_2=0.29

Monte-Carlo simulations

It is generally accepted [1] that homogeneous MF equations are quite inadequate for describing the dynamics of spatially constrained systems. As also addressed in references [1-8] the MF approach cannot take into account the complex phenomena arising from local interactions. The restriction of the dynamics on a low dimensional support has been studied earlier [2,8,20,21] and it was shown that local fluctuations are responsible for driving the system away from MF behavior. To study this we follow references [2,8] and restrict the LLV process on a 2d square lattice support. Each site of the support contains either an X_1 or X_2 particle or it is empty (S). For the reactive steps we consider only nearest neighbor interactions and for the dynamics we use the following Monte-Carlo scheme.

1. At every elementary time step select one site at random.

2. Then, select one of its nearest neighbors at random.

3. Check if these two sites are compatible with any of the reaction of the LLV scheme. If the chosen site is X_1 and the neighbor X_2 then the selected site becomes X_2 with probability k_s. If the chosen site is X_2 and the neighbor S then the selected site becomes S with probability k_1. Finally, if the chosen site is S and the neighbor X_1 then the selected site becomes X_1 with probability k_2.

4. In all other case the lattice remains unchanged.

5. Increase the elementary time by one unit and return to step (1).

One Monte-Carlo step is completed when each lattice site is visited once on average (that is after L^2 elementary steps, where L is the linear lattice size). If the system is initialized from homogeneously random initial conditions then it organizes spontaneously into small local oscillators that are oscillating incoherently. As a results, if we calculate the species concentrations in large spatial scales they seem to attain a constant value but in smaller scales the system appears to oscillate coherently [2,8]. Furthermore, it has been shown that these local oscillators have fractal structure and the fractal analysis can also reveal their characteristic length [8]. In Fig. 3 snapshots of the evolution of the system are given when initialized from homogeneous initial conditions.

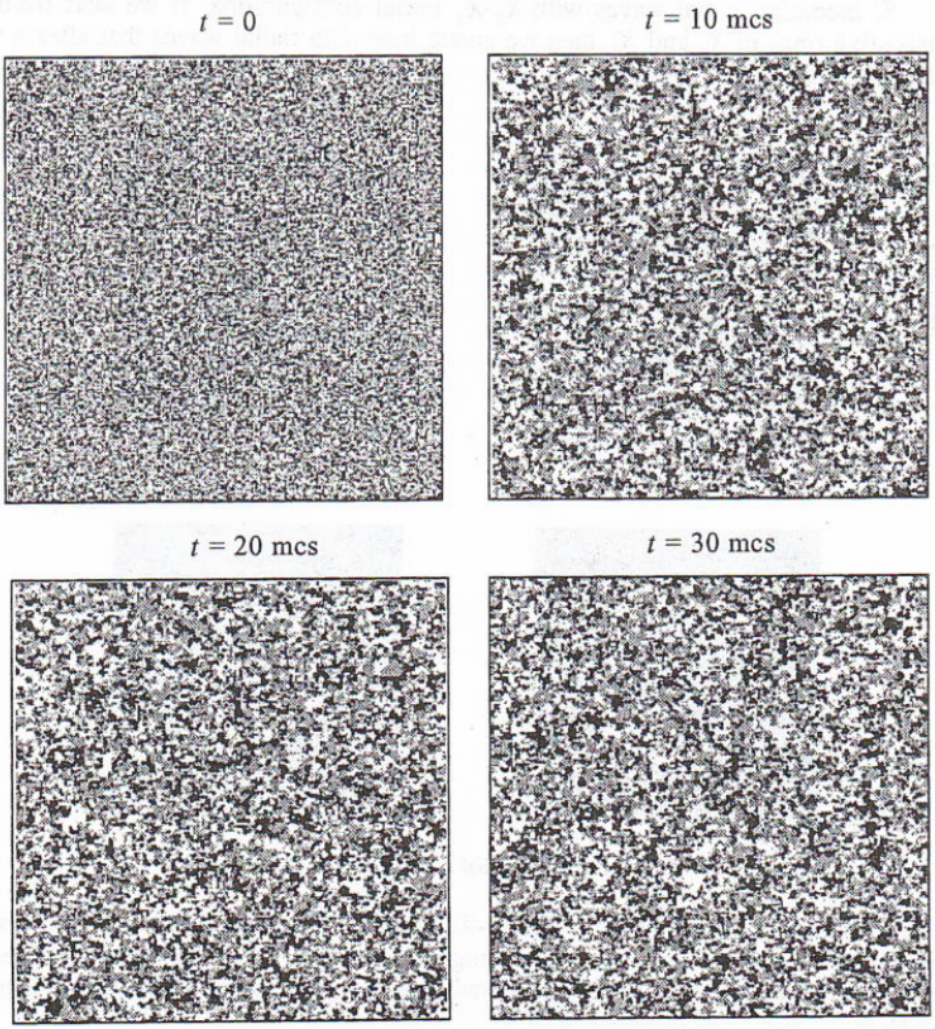

Fig. 3. Evolution of the system for a_1=0.333 and a_2=0.333 (k_1=k_2=k_s=1). X_1 particles are depicted by gray, X_2 by white and empty sites are black. The lattice size is L=200

Waves in the LLV-model

In a recent work [21], some wave solutions have been reported to exist for the LLV-model and furthermore the roughening process of the traveling fronts was extensively studied. In this paper we give a full report of already known and new types of traveling solutions and we also study their collision properties. We work for the case $a_1=a_2=0.333$ since in that domain all the wave fronts demonstrate their most stable behavior. The possible traveling solutions for LLV can be categorized as following.

1. X_1-X_2 linear fronts [21]. In this case the fronts propagate through the empty lattice on constant velocity and the fronts roughen with time. This fronts are unstable and they tend to collapse after some time proportional to their initial width.

2. Random linear front [21]. In this case we have the spontaneous creation of X_1-X_2-S zebra like formations and the self-organized front is moving with constant velocity inside the medium.

3. Random disc [21]. Starting from an initial random disc we have the spontaneous creation of zebra like waves as above that propagate outwards.

4. Spiral wave [21]. If we start in a circular lattice by setting three domains of 120° of X_1, X_2 and S respectively then a fractal spiral wave is created.

5. Incoming radial waves with X_2-X_1 initial configuration. If we start from two consecutive rings of X_2 and X_1 then we create incoming radial waves that after a while collapse into the center (Fig. 4).

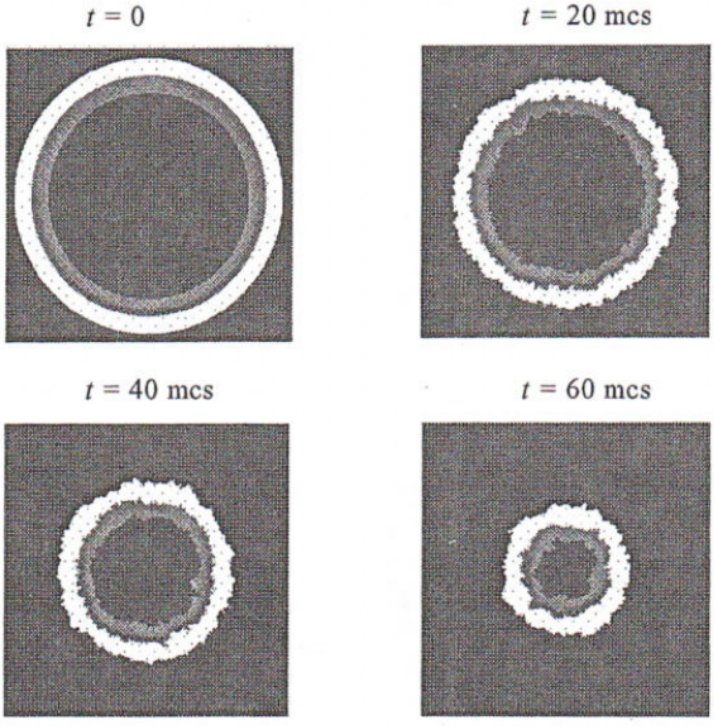

Fig. 4. Incoming radial wave in an L=512 lattice

6. Outgoing radial waves with X_1-X_2 initial configuration. If we transpose the previous configuration then we have outgoing radial waves. These waves are also unstable and collapse after time proportional to the original radial width of the rings (see Fig. 5).

7. Double spiral. Using again a circular lattice and dividing it into 6 areas of X_1, X_2

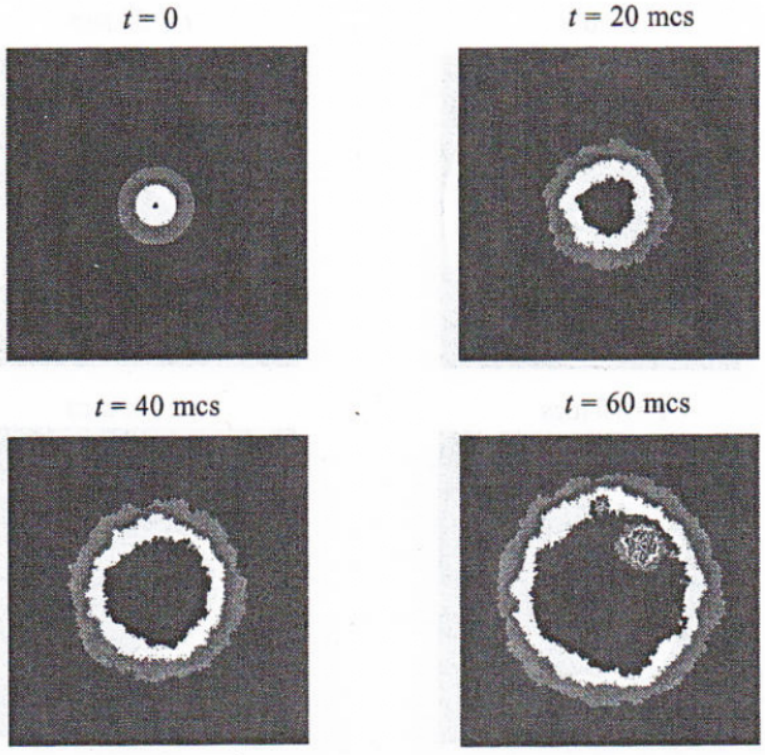

Fig. 5. Outgoing radial wave

and S as in Fig. 6 we may create another spiral wave with more complicated structure than the original one (see Fig. 6). The same is true for spirals of order $3n$.

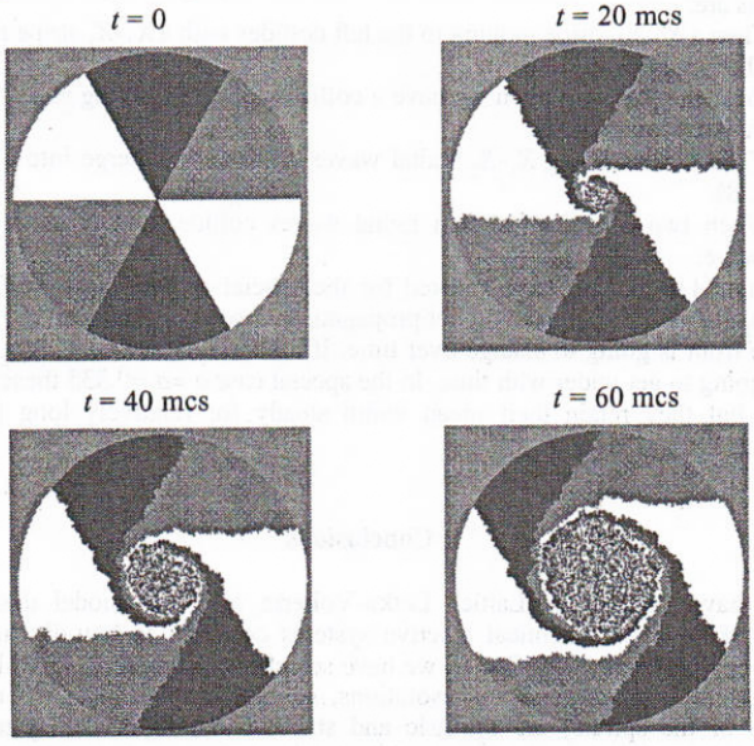

Fig. 6. Double spiral wave

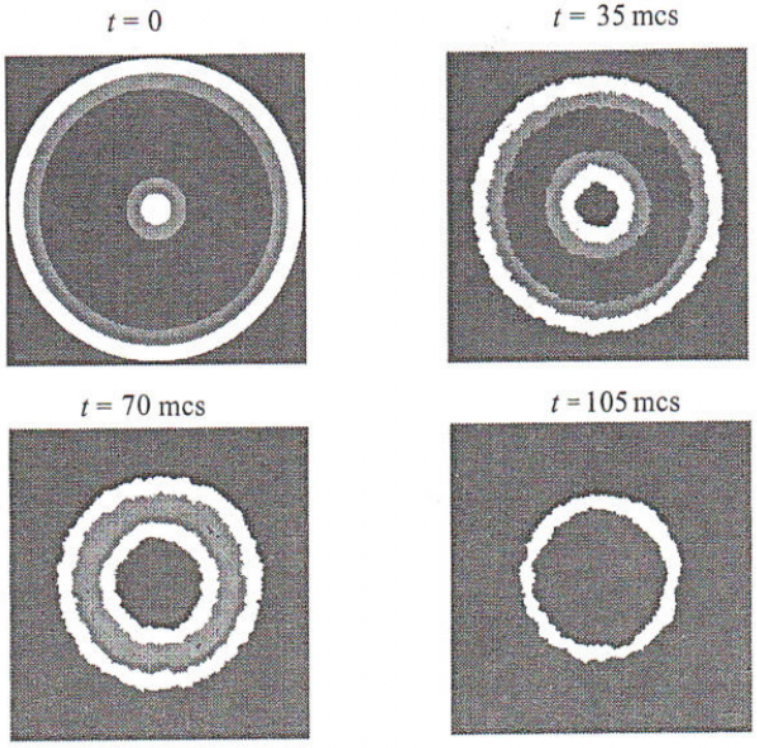

Fig. 7. Incoming-Outgoing collision (L=1024)

We have also studied the collision rules of these types of waves. Our main conclusions are:

• When a X_1-X_2 stripe moving to the left collides with a X_2-X_1 stripe moving to the right they both annihilate.

• The same happens when we have a collision of an incoming radial wave with an outgoing radial wave (Fig. 7).

• When two outgoing X_1-X_2 radial waves collide they merge into a big outgoing wave (Fig. 8).

• When two outgoing random radial waves collide they create a new random outgoing wave.

As noted earlier we have worked for the special case of a_1=a_2=0.333. If we use different a_1 and a_2 then we can still get propagation as seen in Figs 4 and 5. However, the size of the front is going to change over time. If for instance we take a_1>a_2 the X_1 radial region is going to get wider with time. In the special case a_1=a_2=0.333 these radial stripes propagate but they retain their mean width steady for relatively long times (before random fluctuations break them).

Conclusions

We have studied the Lattice Lotka-Volterra as a toy model describing basic properties of nonlinear chemical reactive systems confined to low-dimensionality and low-diffusivity systems. Specifically, we have searched for traveling wave-like solutions. We have found a plethora of such solutions, some of which, (like the random zebra formations or the spirals) are intrinsic and stable solutions of the system appearing spontaneously and being quite stable while others, such as the outgoing and incoming

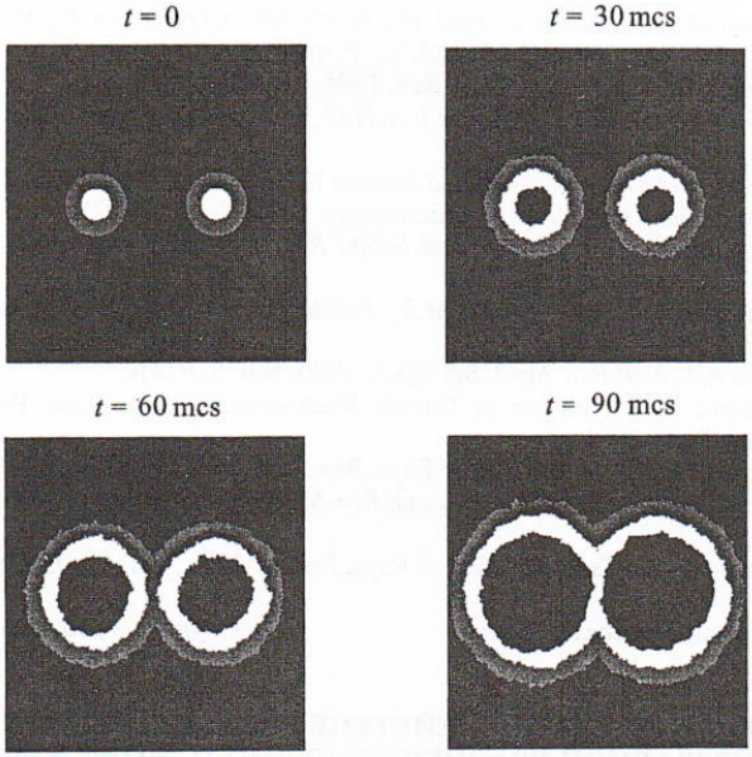

Fig. 8. Outgoing-Outgoing collision (L=1024)

X_1-X_2 solutions are unstable and tend to collapse to more stable solutions. We have also studied the collision rules of such solutions.

It is quite evident from the above discussion that even systems with simple dynamics, such as the LLV, can produce a large variety of dynamical spatiotemporal patterns and are thus good, simple candidate models for analytical and numerical experimentation and for understanding the underlying principles of such complexity before engaging into the analysis of more complicated real-world systems.

Acknowledgments

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References

1. *Nicolis G. and Prigogine I.* Self-organization in Non-equilibrium Systems. Wiley, New York, 1977.
2. *Provata A., Nicolis G. and Baras F.*// J. Chem. Phys. 1999. Vol. 110. P.8361.
3. *Tretyakov A., Provata A. and Nicolis G.* // J. Phys. Chem. 1995. Vol. 99. P. 2770.
4. *Baras F., Vikas F. and Nicolis G.* // Phys. Rev. E. 1999. Vol. 60. P. 3797.
5. *Imbihl R. and G. Ertl* // Chem. Rev. 1995. Vol. 95. P. 697.
6. *Zhdanov V.P.* // Phys. Rev. E. 1999. Vol. 59. P. 6292.
7. *Rose H., Hempel H. and Schimanksy-Geier L.* // Physica A. 1994. Vol. 206. P. 421.
8. *Tsekouras G.A. and Provata A.* // Phys. Rev. E. 2001. Vol. 65. 016204.
9. *Ertl G., Norton P.R. and Rustig J.* // Phys. Rev. Lett. 1982. Vol. 49. P. 177.

10. *Ehsasi M., Matloch M., Frank O., Block J.H., Christmann K., Rys F.S. and Hirschwald W.* // J. Chem. Phys. 1989. Vol. 91. P. 4949.

11. *Imbihl R. and Ertl G.* // Chem. Rev. 1995. Vol. 95. P. 697.

12. *Slinko M., Fink T., Loher T., Madden H.H., Lombardo S.J., Imbihl R. and Ertl G.* // Surface Science. 1992. Vol. 264. P. 157.

13. *Voss C. and Kruse N.* // Applied Surface Science. 1994. Vol. 87/88. P. 127.

14. *Voss C. and Kruse N.* // Ultramicroscopy. 1998. Vol. 73. P. 211.

15. *Hartmann N., Kevrekidis Y. and Imbihl R.* // J. Chem. Phys. 2000. Vol. 112. P. 6795.

16. *Fink Th., Path J.-P., Basset M.R., Imbihl R. and Ertl G.* // Surface Science. 1991. Vol. 245. P. 96.

17. *Lotka A.J., Natl P.* // Acad. Sci. USA. 1920. Vol. 6. P. 410.

18. *Volterra V.* Lecons sur la Theorie Mathematique de la Lutte Pour la Vie. Gauthier-Villars, Paris, 1931.

19. *Picard G. and Johnston T.W.* // Phys. Rev. Lett. 1982. Vol. 48. P. 1610.

20. *Frachebourg L., Krapivsky P.L. and Ben-Naim E.* // Phys. Rev. E. 1996. Vol. 54. P. 6186.

21. *Provata A. and Tsekouras G.A.* // Phys. Rev. E. 2003. Vol. 67. 056602.

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ВОЛНЫ И ИХ ВЗАИМОДЕЙСТВИЕ В МОДЕЛИ РЕШЕТКИ, ОПИСЫВАЕМОЙ УРАВНЕНИЯМИ ЛОТКИ - ВОЛЬТЕРРЫ

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В работе изучается динамика двумерной решетки, которая в приближении среднего поля описывается уравнениями Лотки - Вольтерры. Рассматривается процесс распространения волновых фронтов, появляющихся при задании специальных начальных условий. В зависимости от выбора конфигурации начального состояния система демонстрирует распространение волн различного типа: плоских, радиальных и спиральных.

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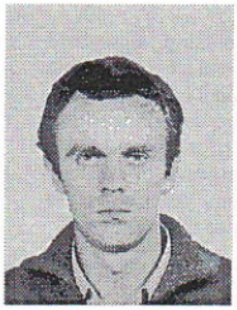

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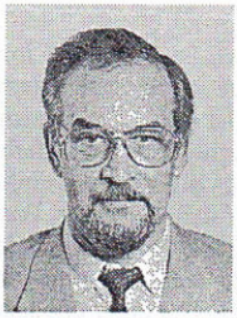

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