# Wave propagation in heterogeneous excitable media

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Heterogeneities deeply affect pulse dynamics in excitable media. In one dimension, spatially periodic variation of the excitation threshold leads to a characteristic dependence of the propagation speed on the modulation period $d$ with a maximum at a certain optimal value $d_{\mathrm{opt}}$. The maximum speed may be larger than the pulse velocity in an effective homogeneous medium. In two dimensions, the geometry and size of heterogeneities determine the wave dynamics. For example, an excitability distribution made of oblique stripes with different angles of inclination can result in a speedup or a slowdown of the pulse. The calculations are carried out with a modified Oregonator model for light-sensitive Belouzov-Zhabotinskii media where a heterogeneous distribution of excitability can be achieved by inhomogeneous illumination. Nevertheless, the results do not depend on the details of the local kinetics, but apply to the general case of excitable media. [S1063-651X(98)05704-3]

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## I. INTRODUCTION

Experimental as well as theoretical investigations on wave propagation in chemical systems are often motivated by their potential role in the understanding of functional aspects in biological systems [1,2]. For example, rotating spiral waves and expanding target patterns studied in the Belousov-Zhabotinskii (BZ) reaction are also observed in many biological systems such as the animal retinas [3], the cytoplasm of frog oocytes [4], or the heart tissue [5]. The cellular structure of living systems, however, gives rise to inhomogeneities and anisotropy not present in homogeneous reaction systems. These properties may play an important role in the behavior of biological systems. An example of how wave propagation can be influenced by heterogeneities is given in the cardiac tissue. Its cellular structure not only causes local variations in wave velocity [5] but also gives rise to propagation failure [6]. In heterogeneous catalysis we find other examples of inhomogeneous active media that may have technical relevance. Here the spectrum reaches from periodically arranged inhomogeneities (e.g., defects) up to randomly distributed catalytically active centers in fixed-bed catalysts. The complex spatiotemporal dynamics of heterogeneous catalytic chemical reactions on single-crystal surfaces have therefore been the subject of intense experimental and modeling research in recent years [7–9]. These investigations have shown that, e.g., controlled surface inhomogeneities can gradually suppress certain types of reaction patterns or act as pacemakers on the catalytic surface [10].

In experiments with BZ media, usually the catalyst is immobilized in a thin gel layer to avoid disturbances of hydrodynamic origin. The interaction of chemical waves with an unexcitable, catalyst-free gap has been studied by artificially introducing a slit into the gel layer [11]. A wave overcomes the gap by diffusion as long as its width is small. Due to the time delay during the tunneling across the gap, the effective propagation velocity of the wave is smaller than in the homogeneous case. There is a critical gap width in a given medium such that gaps with larger width act as an impermeable barrier. In a one-component bistable medium the critical gap width follows from a modified Maxwell condition [12].

The light-sensitive variant of the BZ reaction constitutes an experimental system where the excitability of the medium can be manipulated by the intensity of incident light. For spiral waves a periodic temporal change of the excitability due to external forcing results in mode locking and various resonance effects [14]. A global feedback where the spatial average of the emerging pattern determines the excitation threshold pattern via the incident light can lead to anormal synchronization in a excitable medium with oscillatory defects [15].

Recent experimental investigations in a patterned BZ system prepared by printing the catalyst of the reaction on membranes show that cellular inhomogeneities give rise to global anisotropy in wave propagation, with specific local patterns resulting in various geometries [13]. In such inhomogeneous systems spiral wave sources may appear spontaneously and serve as organizing centers of the surrounding wave activity.

In this paper we study the influence of a heterogeneous distribution of excitability on the dynamics of nonlinear waves. We present numerical results showing the influence of different length scales of heterogeneities on the propagation speed of waves in one and two spatial dimensions.

## II. MODEL

A detailed mechanism of the BZ reaction was proposed by Field, Körös, and Noyes in 1972 [16]. This so-called Field-Körös-Noyes mechanism involves 11 basic reactions among 12 reaction species and was later on reduced by Field and Noyes to five steps among three chemical species: bromous acid ($HBrO_2$) (the autocatalytic variable), bromide ions ($Br^-$) (playing the role of an inhibitor), and the oxidized form of the metal ion catalyst [Me(ox)] (the recovery variable). This kinetic description, known as the three-component Oregonator model, can explain many of the features of the BZ reaction. The model may be further reduced to a two-variable version under the assumption that $Br^-$ always remains in equilibrium with the local instantaneous

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concentration of $HBrO_2$ (a fast process) [17].

In the light-sensitive variant of the BZ reaction the ruthenium-bipyridyl complex is used as a catalyst. Although the chemical changes that occur in the ruthenium-catalyzed BZ reaction under illumination are not known in detail, the Oregonator may be regarded as a first approximation to describe the dynamics on a qualitative level. In the usual scheme of the reaction, the ruthenium-bipyridyl complex promotes the autocatalytic production of the activator $HBrO_2$ only in its reduced and photochemically unexcited state. Once the ruthenium complex becomes photochemically excited, it slowly catalyzes the production of the inhibitor bromide. Externally applied illumination can thus create an additional source of inhibitor $Br^-$ and suppress the excitability of the medium [18]. In order to take into account the photochemically produced $Br^-$, Krug, Pohlmann, and Kuhnert introduced an additional flow term into the equation for the bromide balance. The corresponding system of differential equations (a two-component modified Oregonator) that describes these processes has the form [19]

$$\frac{\partial u}{\partial t}=\frac{1}{\varepsilon}\left(u-u^2-(fv+\phi)\,\frac{u-q}{u+q}\right)+D_u\nabla^2 u,$$

$$\frac{\partial v}{\partial t}=u-v+D_v\nabla^2 v. \tag{1}$$

Here $u$ and $v$ denote the instantaneous local concentrations of bromous acid and the oxidized form of the ruthenium-bipyridyl complex, respectively, scaled to dimensionless quantities using the five reaction steps the Oregonator takes into account and the recipe parameters [20]. $\varepsilon \ll 1$ represents the ratio of time scales of the two variables and is determined by rate constants and chemical concentrations of the reactants. The parameter $q$ depends only on rate constants and has been estimated to be between 0.0002 and 0.002 [21]. The parameter $f$ is related to the stoichiometric coefficient $h$ in the reaction step of the Oregonator scheme that describes the $Br^-$ release by oxidation of malonic and bromalonic acid. The Laplacians $\Delta v$ and $\Delta u$ describe the diffusion of the two species. The ratio of diffusion coefficients $D_v/D_u$ can be estimated from the molecular weights of $HBrO_2$ and the catalyst. In the experiment there is no diffusion of $v$ if the catalyst is immobilized in a gel matrix. The parameter $\phi$ describes the photochemically produced bromide flow. It is, in a first approximation, proportional to the intensity of the incident light. For a fixed value of $f$, $\phi$ controls whether the system is in the oscillatory, the excitable, or the bistable regime.

A heterogeneous distribution of excitability can be achieved by spatial variation of the parameter $\phi$ (which corresponds to a spatially inhomogeneous illumination in the experimental system). High (low) values of $\phi$ result in a medium with high (low) excitation threshold. The length scales of the heterogeneities are imposed on the system by the modulated geometry.

The inherent dynamic length scales of the system depend on the type of pattern under consideration. For pulse propagation they are given by the width of the pulse and the width of the front. These are determined by the parameters of the system, especially by the time scale ratio $\varepsilon$.

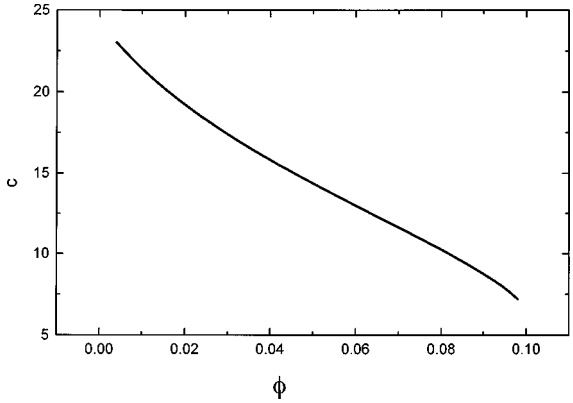


FIG. 1. Nonlinear dependence of pulse velocity on the excitation threshold in a homogeneous medium (with system length $L_{\mathrm{syst}}=200$).

The numerical investigations presented in Sec. III are performed by integrating Eq. (1) in one and two spatial dimensions with no flux boundary conditions. The time derivatives are substituted by differences using an explicit Euler method. The Laplacians are calculated by a five-point discretization, that is, considering the four nearest neighbors of each grid point. The calculations in one spatial dimension are carried out on a vector with up to 26 000 points and grid spacing between $x=0.1$ and 0.0075. A $900\times 280$ array with grid spacing $x=0.1$ is used for the calculations in two spatial dimensions. Convergence of the results with respect to finer discretizations has been tested for all cases. The following model parameters are fixed for all the simulations presented: $\varepsilon=0.004$, $q=0.002$, $f=2.7$, $D_u=1.0$, and $D_v=0.6$.

## III. RESULTS

### A. Traveling pulse in a medium with periodically modulated excitability

A propagating pulse is a solution of system (1) in the locally excitable regime. At a given excitation threshold the pulse adopts a certain profile and propagates with constant velocity. Variations of the excitation threshold lead to changes in the pulse profile and to an increase or decrease of its propagation speed. In a highly excitable medium (low values of $\phi$) broad pulses with high amplitude and high velocity $c$ are favored. The curve $c(\phi)$ presented in Fig. 1 shows a nonlinear decrease in pulse velocity with increasing excitation threshold. At the same time the amplitude and the width of the pulse decrease. For $\phi$ values larger than 0.1 pulse propagation becomes unstable.

Our numerical investigations in one spatial dimension focus on a pulse traveling in a heterogeneous system with periodically changed excitability generated according to

$$\phi(x)=\begin{cases}\phi_1 & \text{for } nd<x\leqslant(n+\frac{1}{2})d\\ \phi_2 & \text{for } (n+\frac{1}{2})d<x\leqslant(n+1)d,\end{cases} \tag{2}$$

with $n=1,2,\ldots$ . Here $\phi_1<\phi_2$ and the characteristic size of the heterogeneity is determined by the modulation period $d$ (see Fig. 2). Thus half of the system has a high and the other half a low excitation threshold. In the range of the chosen parameter values the system always remains in the

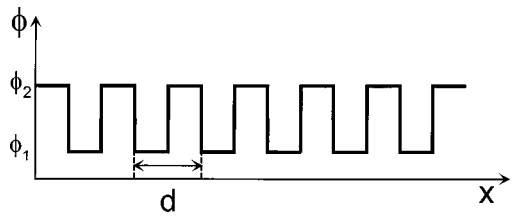


FIG. 2. Spatially periodic variation of excitability. The amplitude $A=(\phi_2-\phi_1)/2$ and the modulation period $d$ define the characteristic size of the heterogeneity.

excitable regime. Let us introduce an effective homogeneous medium with a constant excitation threshold according to

$$\phi_{\mathrm{hom}}=\frac{\phi_1+\phi_2}{2}. \tag{3}$$

A pulse profile corresponding to this effective medium is used as the initial distribution. As soon as the pulse encounters a change in the excitation threshold it adapts to the new $\phi$ level. The average velocity of the pulse is detected for increasing values of $d$, i.e., for increasing size of the heterogeneity. The results are shown in Fig. 3. For small modulation wavelength the propagation speed increases and reaches a maximum at an ''optimal'' size $d_{\mathrm{opt}}$. For wavelengths $d>d_{\mathrm{opt}}$ the velocity decreases. The optimal wavelength depends on the chosen parameters, especially on the time scale ratio $\varepsilon$ that determines the dynamic length scales of the system. For an increasing value of $\varepsilon$ the width of the pulse decreases while the width of the front increases. For such pulses $d_{\mathrm{opt}}$ shifts to larger values that, however, are still smaller than the corresponding dynamic length scales of the system. As follows from Fig. 3, the propagation speed at the optimal wavelength can be even higher than the pulse velocity in the corresponding effective homogeneous medium $c_{\mathrm{hom}}=c(\varepsilon,f,(\phi_1+\phi_2)/2)$. As a measure for this difference we define the ratio

$$\beta=\frac{c(d_{\mathrm{opt}})}{c_{\mathrm{hom}}}, \tag{4}$$

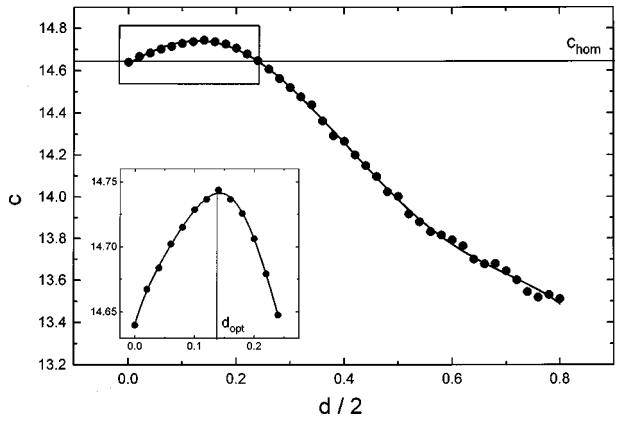


FIG. 3. Pulse velocity in a medium with periodic variation of excitability according to Fig. 2 with $\phi_1=0.006$ and $\phi_2=0.09$. The curve exhibits a maximum at $d_{\mathrm{opt}}=0.14$ that is smaller than the front width $L_{\mathrm{front}}=0.54$ and the pulse width $L_{\mathrm{pulse}}=1.82$. The maximum velocity is higher than the velocity $c_{\mathrm{hom}}$ in the corresponding homogeneous effective medium.

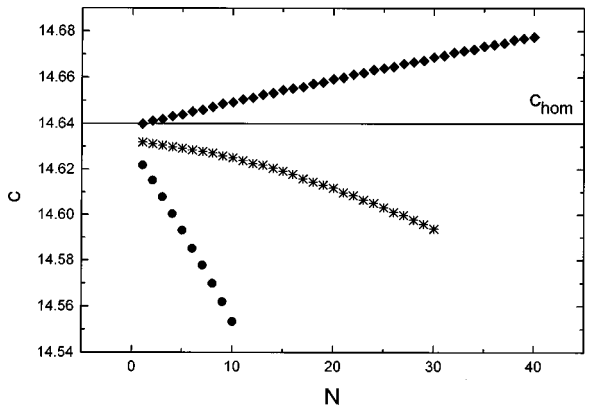


FIG. 4. Pulse velocity in a system including an increasing number $N$ of modulation periods. The model parameters are $\phi_1=0.006$, $\phi_2=0.09$, and $L_{\mathrm{syst}}=80$. The propagation speed increases for $d=0.14=d_{\mathrm{opt}}$ (♦) and decreases for $d=0.28>d_{\mathrm{opt}}$ (*) and $d=0.5\gg d_{\mathrm{opt}}$ (●).

which depends on the parameters of the medium and on the amplitude of the spatial modulation. Decreasing values of the time scale ratio $\varepsilon$ result in an increase of $\beta$.

In order to get more insight into the above-described behavior of pulse velocity we performed further numerical investigations on a pulse traveling in a homogeneous system that includes an inhomogeneous area with increasing size. The inhomogeneous area consists of an increasing number of cells (modulation periods) with length $d$, i.e., its size is $N^*d$ (compare Fig. 2). Some results are shown in Fig. 4. If we choose $d=d_{\mathrm{opt}}$ for a given set of parameters, the pulse velocity increases with increasing number of cells $N$. For $d>d_{\mathrm{opt}}$ and $d\gg d_{\mathrm{opt}}$ the propagation speed decreases with increasing $N$. The decrease in velocity becomes steeper for higher values of $d>d_{\mathrm{opt}}$. These results show that already one single heterogeneity with size $d$ (one modulation period) results in an increase (for $d\leqslant d_{\mathrm{opt}}$) or a decrease (for $d>d_{\mathrm{opt}}$) of pulse velocity and that the effect changes almost linearly with $N$. From the nearly linear increase of the velocity with $N$ it is evident that the maximum in the $c(d)$ dependence does not result from a resonancelike effect. The reason for this maximum is rather the incomplete adaptation of the pulse profile to the local properties of the inhomogeneous medium during propagation. When the pulse is traveling a distance equal to $2L$, with $L$ at excitability $\phi_1$ and $L$ at excitability $\phi_2$, there is an asymmetry between the up-sweep and the down-sweep case. The transition of a pulse from a low excitation threshold to a high one is faster than in the opposite case: For the $\phi_1\rightarrow\phi_2$ transition we get an advance and in the opposite case a delay in the time compared to $\tau_{\mathrm{hom}}=L[c^{-1}(\phi_1)+c^{-1}(\phi_2)]$. Here $\tau_{\mathrm{hom}}$ is the time the pulse would need to travel the distance $2L$ *neglecting* the transition between the different $\phi$ levels. Figure 5 presents the difference in propagation time $\tau_{\mathrm{rel}}$ for a sequence $\phi_2\rightarrow\phi_1\rightarrow\phi_2$ that corresponds to one modulation period $d$. The calculations reveal a pronounced minimum close to $d=d_{\mathrm{opt}}$. A similar dependence was obtained for the sequence $\phi_1\rightarrow\phi_2\rightarrow\phi_1$.

To summarize, in a medium with periodically changing excitation threshold the pulse can completely adapt its profile only if the modulation wavelength is large enough. At small

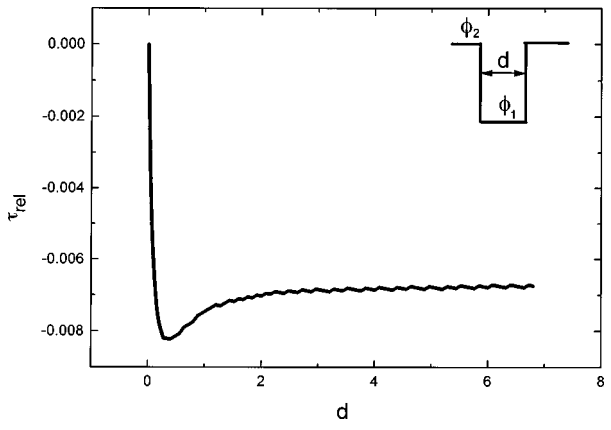


FIG. 5. Relaxation time $\tau_{\mathrm{rel}}=\tau-\tau_{\mathrm{hom}}=\tau-L[c^{-1}(\phi_1)+c^{-1}(\phi_2)]$ of a pulse traveling in a medium with excitation threshold according to $\phi_1=0.006$, which includes an area of size $d$ with excitation threshold according to $\phi_2=0.09$.

wavelength the pulse does not have enough time to completely adapt its profile. For a transition from a low to a high excitation threshold it can better adapt it than for the reversed transition. This periodic interplay of a fast and a slow transition can lead to an increase of the propagation speed for a small modulation wavelength. Its maximum can be even higher than the propagation speed in the corresponding homogeneous medium.

### B. Plane waves in two-dimensional heterogeneous excitable media

A second spatial dimension offers additional possibilities for a pulse to interact with an inhomogeneous distribution of excitability. For example, the pulse can avoid areas with a high excitation threshold. Therefore, the wave dynamics sensitively depends on the geometry of the heterogeneity imposed on the system.

We study the influence of heterogeneous distributions of excitability with different geometries on the propagation speed of a plane wave. The system we investigate consists of three parts: the areas at the beginning and at the end of the system have an excitation threshold corresponding to the homogeneous effective medium; the middle area consists of a heterogeneous distribution of excitation threshold with different geometries (see Fig. 6). Velocity detectors were placed in the homogeneous areas at the beginning and at the end of the system in order to get a more accurate determination of

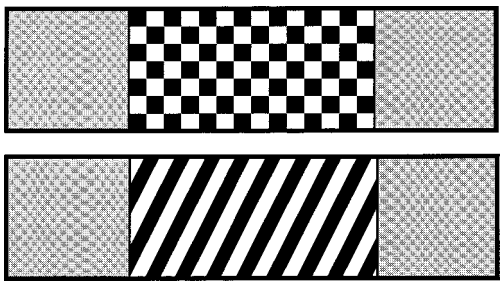

FIG. 6. Excitability patterns used for numerical investigations in two spatial dimensions. The excitation threshold is assigned as follows: black, $\phi_2=0.09$; white, $\phi_1=0.006$; and gray, $(\phi_1+\phi_2)/2$.

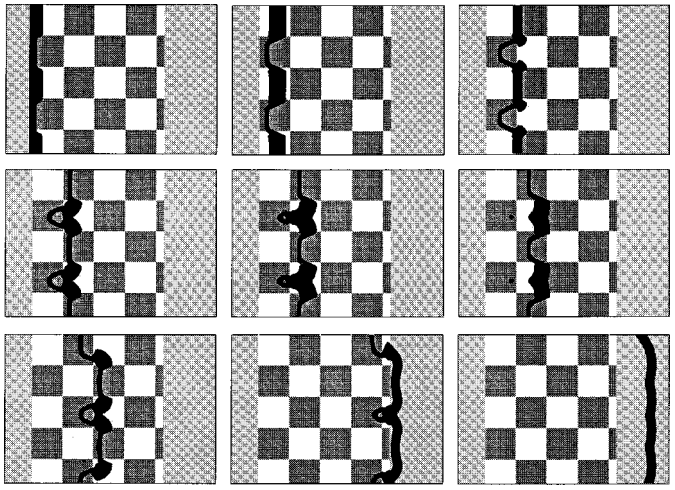

FIG. 7. Time sequence of a plane wave traveling through a medium with a heterogeneous distribution according to Fig. 6(a). The gray-scale code displays high amplitudes of activator concentrations in black. Dark squares in the inhomogeneous area denote high and light squares denote low excitation threshold. The size of the squares is $d=5.0$.

wave velocity (in these areas the wave is straightened).

A time sequence of a plane wave traveling through a medium with a checkerboard type of heterogeneity in the middle area is depicted in Fig. 7. The gray-scale code used for the presentation of the numerical results displays high amplitudes of activator concentrations in black. Dark squares in the inhomogeneous area denote a high excitation threshold and light squares denote a low excitation threshold. The wave starts in the homogeneous area at the beginning of the system. It becomes distorted as soon as it encounters the first squares of the heterogeneous area; the wave parts in the dark squares are left behind, while those in the light squares widen and travel faster. When the fast wave parts encounter the next dark square they can ''walk'' around this area of low excitability by moving through the high excitable thin channel that is formed by the corners of two consecutive dark squares. The wave parts that thus emerge in the light squares have different orientation from the initial plane wave. The fast propagation of these wave parts results in an increasing curvature of the wave in the dark squares. The slow wave parts get cut off and disappear as soon as the curvature becomes overcritical. The above-described procedure repeats as soon as the wave encounters the next squares, i.e., the wave performs a periodic motion.

When the different wave parts leave the heterogeneous area they merge into one distorted wave that is smoothed due to curvature effects. The velocity of the wave is mainly determined by the interplay between the fast and the slow wave parts in the heterogeneous area. This interplay is influenced by the size of the squares, i.e., the length scale of the heterogeneity. Figure 8 presents the wave velocity with increasing square size. It shows that an increasing length scale of a checkerboard type of heterogeneity leads to wave velocities far above the velocity in the homogeneous system.

Another type of heterogeneity that can lead to interesting effects concerning wave propagation is a composition of oblique stripes with different angles of inclination $\alpha$. Figure 9 presents time sequences of a plane wave traveling through a

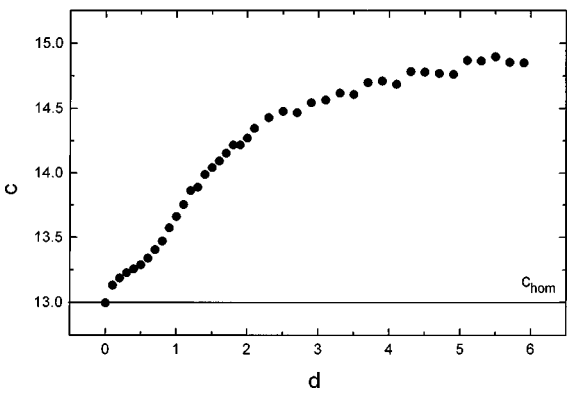


FIG. 8. Pulse velocity obtained for the situation displayed in Fig. 7. $d$ denotes the size of the squares.

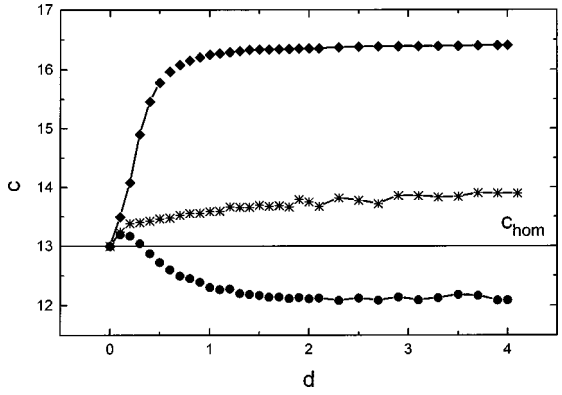


FIG. 10. Pulse velocity obtained for the situations displayed in Fig. 7. $d$ denotes the width of the stripes. $\alpha=80$ (♦), $\alpha=45$ (∗), and $\alpha=20$ (●).

medium including oblique stripes with three different inclinations. The wave again starts in the homogeneous part of the system and becomes distorted when it enters the striped area. The wave parts in the dark stripes are left behind, whereas those in the light parts widen and travel faster along the stripes. This leads to the stretching of the wave parts in the dark stripes. The extent of this wave stretching is mainly determined by the inclination of the stripes. Steep stripes lead to a strong stretching of the slow wave parts, which lasts as long as the angle between the wave parts in the light and in the dark stripes has reached a minimum (slow period). In this situation diffusion can act optimally from all sides. Thus the velocity of the wave parts that formed the cusp is increased and the wave is straightened (fast period). At this point the whole procedure repeats, i.e., the wave performs a periodic motion that consists of short-lasting fast and long-lasting slow periods [see Fig. 9(a)].

Flat stripes lead to a slight stretching of the slow wave parts when the wave enters the inhomogeneous area. This procedure is finished as soon as the wave has completely adapted to the inhomogeneity. The wave now propagates with constant velocity up to the end of the inhomogeneous area [see Figs. 10(b) and 10(c)].

As soon as the wave parts leave the heterogeneous area curvature effects act towards the straightening of the wave. The average wave velocity sensitively depends on the duration of the described fast and slow periods (steep stripes) or on the motion of the fast wave parts (flat stripes). This involves a dependence on the length scale of the heterogeneity, which is denoted by the width of the stripes. Figure 10 depicts the wave velocity with increasing stripe width. Here the difference between the steep and flat stripes becomes obvious: Steep stripes lead to a slowdown and flat stripes to a speedup of the wave. The reason for this behavior can be found in the above-described motion of the wave. For steep stripes, the duration of the slow period (stretching of the wave in the dark stripes) increases for a larger stripe width and causes a decrease of the average wave velocity beyond the value in the homogeneous system. Vertical stripes ($\alpha=0$) correspond to the situation of the one-dimensional pulse described in Sec. III A, i.e., we expect to find an optimal stripe width $d_{\mathrm{opt}}$ where the wave velocity reaches a maximum. Figure 10 shows that such a behavior is also found for $\alpha=20$. For flat stripes, the motion of the wave is hindered by the slow wave parts that are dragged behind by the fast ones. For increasing stripe width the fast wave parts can move more freely and thus increase the average velocity of the wave up to values above the homogenous velocity.

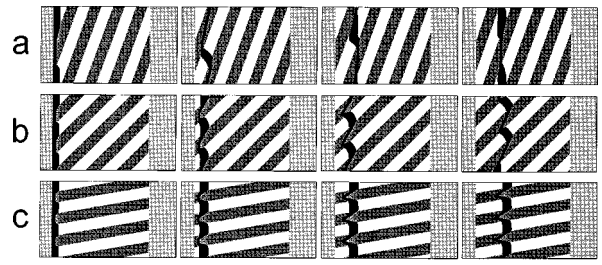


FIG. 9. Time sequences of a plane wave traveling through a medium including oblique stripes with three different inclinations. The gray-scale code displays high amplitudes of activator concentrations in black. Dark stripes in the inhomogeneous area denote high and light stripes denote low excitation threshold. The width of the stripes is $d=4.0$. (a) $\alpha=20$, (b) $\alpha=45$, and (c) $\alpha=80$.

## IV. DISCUSSION

In excitable media spatiotemporal variation of the medium's properties provides a rich set of possibilities for affecting and controlling pulse dynamics. A good candidate for the experimental investigation of those effects are light-sensitive BZ media. Therefore, our calculations are based on a modified Oregonator model for the ruthenium-catalyzed BZ system. The model includes an additional term $\phi$ in the balance of the inhibitor bromide that accounts for its photochemical production. In a first approximation $\phi$ is proportional to the local intensity of incident light. Because $\phi$ affects the excitation threshold, a required spatiotemporal distribution of excitability may be generated by inhomogeneous illumination. Nevertheless, our main results do not depend on the details of the reaction kinetics, but describe the generic behavior in excitable media.

We have studied in this paper pulse propagation in a medium whose excitation threshold varies periodically in space. In one dimension, most striking is the observation of a maximum pulse velocity for a certain spatial modulation period $d_{\mathrm{opt}}$ when all other parameters are fixed, especially the overall portion of weakly and strongly excitable areas of the me-

dium. We argue that the adaptation of the pulse profile to the local excitability is the reason for the observed velocity dependence on the modulation period.

In two spatial dimensions, in addition to the size, the geometry of the heterogenization plays an important role. The second spatial dimension offers the possibility to avoid a weakly excitable area. Again we find that the pulse velocity depends nontrivially on $d$.

The existence of an optimal heterogenization length may be of interest for catalytic reactions on composite catalyst surfaces. Another interesting example provides fixed-bed catalysts. In contrast to the situation considered in this paper, in a fixed-bed catalyst the active sites are distributed randomly throughout the medium. The distance between neighboring sites fluctuates around a certain mean value $\langle d \rangle$. To be closer to this situation, we randomly arranged weakly and strongly excitable segments of widths $d$. Then we determined the pulse velocity in this stochastically heterogeneous medium. Averaging over a large number of random realizations, we found a similar dependence of the pulse speed on $d$ as in the case of periodic modulation. The curve looks qualitatively like Fig. 3; however, it is shifted to smaller values because of $\langle d \rangle > d$. Details will be reported elsewhere.

## ACKNOWLEDGMENTS

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