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A Reaction–Diffusion Equation for a Cyclic System with Three Components

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The one-dimensional reaction-diffusion equations for the process

$$A+B\rightarrow 2A, \qquad B+C\rightarrow 2B, \qquad C+A\rightarrow 2C \qquad \text{(D)}$$

are extended to include the counteracting reactions

$$A+2B\rightarrow 3B, \qquad B+2C\rightarrow 3C, \qquad C+2A\rightarrow 3A \qquad \text{(R)}$$

which have a reaction rate α relative to the direct process (D). This process can be seen as a three-component version of the reaction which is described by the Fisher–Kolmogorov equation. The fixed points of the equations are studied as a function of α. It is shown that the equations admit solutions which consist of a series of traveling fronts. Other solutions exist which are traveling periodic waves. A very remarkable fact is that for these waves exact expressions can be constructed.

KEY WORDS: Fisher–Kolmogorov equation; traveling fronts; fixed points; population dynamics; bifurcations; stability.

1. THE ABC MODEL

Reaction–diffusion processes and pattern formation have been widely studied in physics and chemistry, as well as in mathematics and biology. References 1–4 give an almost exhaustive description of the activities in this field and of the state of the art. In general, criteria for the behavior of a system do not exist and for each new system it is necessary to develop new methods in order to detect its characteristic properties. This is particulary true when the governing equations have more than one component.

In the present paper we will give an example of such a system, which we believe shows sufficiently many new aspects to justify its presentation.

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Consider an infinite n-dimensional coordinate space, in which three species A, B, and C are competing in a way described by the direct reaction

$$A+B\to 2A, \qquad B+C\to 2B, \qquad C+A\to 2C \tag{D}$$

In words: when two individuals A and B meet, B is converted into A. The species B, however, tries to survive by conquering C and similarly C beats A. This reaction is similar to the cyclical "Rock-paper-scissor's game," of which the first biological example has been found recently.[5, 6] When diffusion is added, we arrive at a system of equations which can be seen as a generalization of the Fisher–Kolmogorov equation. This well-studied equation is obtained by considering the reaction $A+B\to 2A$, with a diffusion term. By taking the concentration of $C=0$, we see that (D) then reduces to this equation.

It will be shown that the reaction part of the equation corresponding to (D) (a system of ordinary differential equations which is obtained by ignoring the diffusion term) has an integral of motion. In terms of ordinary differential equations, this is a structurally unstable situation. It is remedied by introducing the reverse reaction

$$A+2B\to 3B, \qquad B+2C\to 3C, \qquad C+2A\to 3A \tag{R}$$

which has the following interpretation. The B-population, in an effort to defend itself against A, changes its strategy, and decides sometimes to travel in pairs, so that a single A can be overcome in the reaction $A+2B\to 3B$. The C and A populations, however, adopt the same strategy, so that as a result the system is described by the reactions (D) and (R).

In this paper we will study the equation derived from (D) and (R), emphasizing two aspects: its similarity with the Fisher–Kolmogorov equation and the qualitative effect of adding reaction (R) to the (unstable) reaction (D).

The three reaction constants of the reactions (D) are k_{D} and those of the reactions (R) are also given equal values k_{R}. The diffusion constants of the three species are equal to D. Since in the reactions (D) and (R) the number of individuals does not change, the sum of the population densities $S=A+B+C$ varies only because of migration:

$$\frac{\partial S}{\partial t}=D\,\Delta S \tag{1.1}$$

In order to simplify the problem we will restrict ourselves to the case in which S has spread uniformly and therefore also has become constant in time $S=S_0$. We now introduce S_0 as a new unit of concentration,

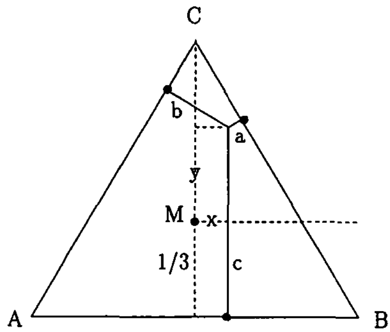

Fig. 1. Representation of A, B, and C as a point of an equilateral triangle of unit height. The Cartesian coordinates x and y are also shown. For typographical reasons we write a, b, c instead of A, B, C.

$\tau = 1/k_D S_0$ as a new unit of time, and $l = \sqrt{D/k_D S_0}$ as a new unit of length. With $\alpha = k_R \tau S_0^2$ as a new measure for the reaction constant of the reactions (R), the reaction–diffusion equations become in dimensionless variables

$$\begin{aligned} \frac{\partial A}{\partial t} &= A(B-C) + \alpha A(AC - B^2) + \Delta A \\ \frac{\partial B}{\partial t} &= B(C-A) + \alpha B(BA - C^2) + \Delta B \\ \frac{\partial C}{\partial t} &= C(A-B) + \alpha C(CB - A^2) + \Delta C \end{aligned} \tag{1.2}$$

These equations are to be studied under the conditions

$$A + B + C = 1, \qquad A, B, C > 0 \tag{1.3}$$

At a certain moment and at a given point in space the values of A, B, and C will be represented by the altitudes of a point inside an equilateral triangle of unit height, as shown in Fig. 1. From now on we will also impose the further restriction to one unbounded space-dimension and we will denote the coordinate by u.

Condition (1.3) is automatically satisfied when we introduce Cartesian coordinates x and y (Fig. 1) and write A, B, and C as

$$A = \tfrac{1}{3} - \tfrac{1}{2}\sqrt{3}\,x - \tfrac{1}{2}y, \qquad B = \tfrac{1}{3} + \tfrac{1}{2}\sqrt{3}\,x - \tfrac{1}{2}y, \qquad C = \tfrac{1}{3} + y \tag{1.4}$$

In terms of these variables the reaction–diffusion equations (1.2) can be written in a form in which the vector field describing the reaction is separated into a source-free and a rotation-free part:

$$\frac{\partial^2 x(u,t)}{\partial u^2}=\frac{\partial x}{\partial t}+f(\alpha)\frac{\partial P}{\partial y}-\alpha\frac{\partial V}{\partial x}$$
$$\frac{\partial^2 y(u,t)}{\partial u^2}=\frac{\partial y}{\partial t}-f(\alpha)\frac{\partial P}{\partial x}-\alpha\frac{\partial V}{\partial y} \tag{1.5}$$

where f is an abbreviation for

$$f(\alpha)=\frac{2}{\sqrt{3}}\left(1-\frac{\alpha}{2}\right) \tag{1.6}$$

The function $P=ABC$ is the product of the three concentrations, which in Cartesian coordinates becomes equal to

$$P(x,y)=\tfrac{1}{27}-\tfrac{1}{4}(x^2+y^2)-\tfrac{3}{4}x^2y+\tfrac{1}{4}y^3 \tag{1.7}$$

while the potential is given by

$$V(x,y)=\tfrac{1}{12}(x^2+y^2)-\tfrac{1}{4}x^2y+\tfrac{1}{12}y^3-\tfrac{3}{16}(x^2+y^2)^2 \tag{1.8}$$

By writing the equations in the form (1.5) the invariance under a cyclic permutation can still be recognized, because $P(x, y)$ and $V(x, y)$ are simple functions of the invariant polynomials x^2+y^2 and $y(3x^2-y^2)$.

The function $P(x, y)$, which is the product of the three altitudes of a point inside an equilateral triangle, has some interesting properties. It satisfies $\Delta P(x, y)=-1$ and $P(x, y)=0$ on the boundary of the triangle. Therefore, it is the solution of the corresponding electrostatic problem. Also, it gives the mean exit time of a random walker to escape from an equilateral triangle.[7]

Singular points are defined as those values of (A, B, C) for which the three reaction terms in the r.h.s. of (1.2) simultaneously vanish. It is clear that this happens in the corners $A=(1, 0, 0)$, $B=(0, 1, 0)$ and $C=(0, 0, 1)$ and also in the midpoint $M=(1/3, 1/3, 1/3)$. With some simple algebraic manipulations it can be shown that there are no other singular points lying strictly inside the triangle.

For $\alpha>1$ there are, however, three other singular points, one on each side. On the AB-side this point is $T=(1-1/\alpha, 1/\alpha, 0)$. For $\alpha=1$ it appears at B. With increasing α it then moves toward A, which is approached for $\alpha\to\infty$. The other fixed points R and S, which also occur only for $\alpha>1$, are obtained from T by rotations over $\pm 2\pi/3$ around M.

Having found the solutions which are constant in space and time, we must also answer the question as to their stability under small perturbations and how this changes with α. This will be done in the next section.

2. THE SINGULAR SOLUTIONS AND THEIR STABILITY

The Centre point *M*. Keeping only the terms in (1.5) which are linear in x and in y, the general solution can be constructed in the standard way.

An arbitrary bounded Fourier component, written as

$$(x(u, t), y(u, t))^T = e^{iku + \lambda t}(x_0, y_0)^T \tag{2.1}$$

with k real, is a solution only if $\lambda = \lambda_+$ or $\lambda = \lambda_-$, where

$$\lambda_\pm = \frac{\alpha}{6} - k^2 \pm \frac{i}{2} f(\alpha) \tag{2.2}$$

From (2.2) it follows that M is stable when $\alpha < 0$ and unstable when $\alpha > 0$, since we can then find values of k such that $\mathrm{Re}\,\lambda_\pm = \alpha/6 - k^2 > 0$.

The Corners *A*, *B*, and *C*. We now linearize (1.5) in one of the corners, for which we take $B = (1/\sqrt{3}, -1/3)$. Defining w and z by $x = 1/\sqrt{3} + w$, $y = -1/3 + z$, an arbitrary bounded Fourier component, written as

$$(w(u, t), z(u, t))^T = e^{iku + \lambda t}(w_0, z_0)^T \tag{2.3}$$

with k real, is a solution only if $\lambda = \lambda_+$ or $\lambda = \lambda_-$, where

$$\lambda_+ = 1 - \alpha - k^2 \qquad \text{and} \quad \lambda_- = -1 - k^2 \tag{2.4}$$

From (2.4) it follows that B is stable when $\alpha > 1$ and unstable when $\alpha < 1$.

The Side Points *R*, *S*, and *T*. For $\alpha > 1$ there are three additional singular points R, S, and T on the sides of the state triangle. The Cartesian coordinates of the point T on the AB side are $x_T = f(\alpha)/\alpha$ and $y_T = -1/3$. Note that for $\alpha \to 1$ the point T approaches B. Linearizing the equations (1.5) around this point in the same way as in the above cases, we find

$$\lambda_+ = 1 - \frac{1}{\alpha} - k^2 \qquad \text{and} \quad \lambda_- = -k^2 - \frac{1}{\alpha}\left[\left(\alpha - \frac{3}{2}\right)^2 + \frac{3}{4}\right] \tag{2.5}$$

Since $\alpha > 1$, it follows from (2.5) that R, S, and T are unstable.

Summing up, we see that M loses stability at $\alpha = 0$. The corner points are unstable for $\alpha < 1$. At $\alpha = 1$ these points become stable and the unstable

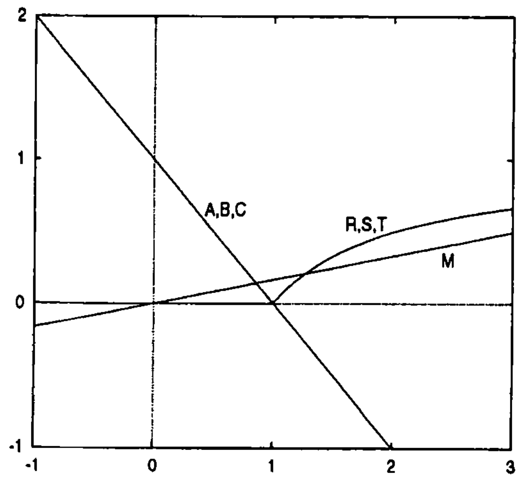

Fig. 2. Stability of the various singular points. Re λ vs. α.

side points are born. This is illustrated in Fig. 2, where we have plotted the real part of the largest eigenvalue for $k=0$ versus α.

3. THE DIRECT REACTION (D) ($\alpha=0$)

In this section we will consider only the direct reaction (D), so that we put $\alpha=0$. In this case (1.5) becomes

$$\begin{aligned}\frac{\partial^2 x(u,t)}{\partial u^2}&=\frac{\partial x}{\partial t}+\frac{2}{\sqrt{3}}\frac{\partial P}{\partial y}\\ \frac{\partial^2 y(u,t)}{\partial u^2}&=\frac{\partial y}{\partial t}-\frac{2}{\sqrt{3}}\frac{\partial P}{\partial x}\end{aligned} \tag{3.1}$$

3.1. Uniform Solutions

We first consider solutions which are uniform in space. They satisfy the ordinary differential equations

$$\begin{aligned}\frac{dx(t)}{dt}&=-\frac{2}{\sqrt{3}}\frac{\partial P}{\partial y}=\frac{1}{\sqrt{3}}y+\frac{\sqrt{3}}{2}(x^2-y^2)\\ \frac{dy(t)}{dt}&=\frac{2}{\sqrt{3}}\frac{\partial P}{\partial x}=-\frac{1}{\sqrt{3}}x-\sqrt{3}\,xy\end{aligned} \tag{3.2}$$

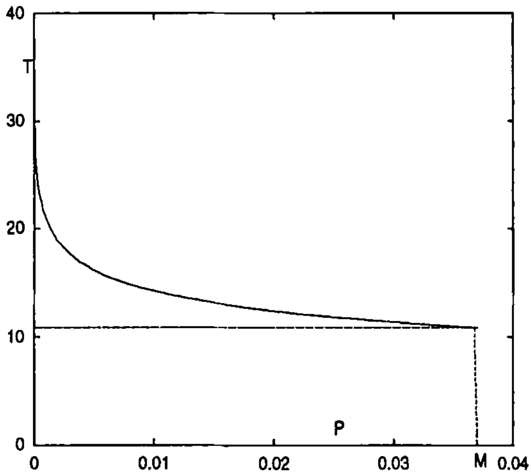

Fig. 3. Period of uniform solutions as a function of P for $\alpha = 0$.

System (3.2) is Hamiltonian, with solutions lying on the closed curves

$$P = ABC = \text{const} = P_0 \tag{3.3}$$

All solutions within the triangle (the only part of the phase space which is of interest to us) are periodic. An expression for the period of an orbit can also be given, but we preferred a numerical calculation. The resulting period T as a function of P_0 is shown in Fig. 3.

For orbits close to the boundary of the triangle, i.e., for $P \approx 0$, the period tends to infinity. For $P \approx 1/27$ the orbits are almost circular and the period is found to be $T \approx 2\pi \sqrt{3}$. We will now consider the stability of the solutions of (3.2), which we denote by $(x_P(t), y_P(t))$, where $P = ABC$ is conserved and $0 < P < 1/27$. For this purpose we consider a slightly perturbed solution $(x_P(t) + w(u, t), y_P(t) + z(u, t))$ of (3.1). Substitution into (3.1) and linearizing in w and z gives

$$\frac{\partial^2}{\partial u^2}\begin{pmatrix} w \\ z \end{pmatrix} = \frac{\partial}{\partial t}\begin{pmatrix} w \\ z \end{pmatrix} + M(t)\begin{pmatrix} w \\ z \end{pmatrix} \tag{3.4}$$

where $M(t)$ is given by

$$M(t) = \begin{pmatrix} -\sqrt{3}\,x & -\dfrac{1}{\sqrt{3}} + \sqrt{3}\,y \\ \dfrac{1}{\sqrt{3}} + \sqrt{3}\,y & \sqrt{3}\,x \end{pmatrix} \tag{3.5}$$

and where we have written (x, y) for $(x_P(t), y_P(t))$. It is sufficient to investigate the stability of periodic perturbations. If therefore we write

$$\begin{pmatrix} w(u,t) \\ z(u,t) \end{pmatrix} = e^{iku} \begin{pmatrix} w(t) \\ z(t) \end{pmatrix} \tag{3.6}$$

Eq. (3.4) becomes

$$\frac{d}{dt} \begin{pmatrix} w(t) \\ z(t) \end{pmatrix} = A(t) \begin{pmatrix} w(t) \\ z(t) \end{pmatrix} \tag{3.7}$$

where now

$$A(t) = \begin{pmatrix} -k^2 + \sqrt{3}\,x & \dfrac{1}{\sqrt{3}} - \sqrt{3}\,y \\ -\dfrac{1}{\sqrt{3}} - \sqrt{3}\,y & -k^2 - \sqrt{3}\,x \end{pmatrix} \tag{3.8}$$

Defining the 2×2 matrix $R(t)$ by

$$\frac{dR(t)}{dt} = A(t)\,R(t) \qquad \text{and} \qquad R(0) = I \tag{3.9}$$

the general solution of (3.7) can be written as

$$\begin{pmatrix} w(t) \\ z(t) \end{pmatrix} = R(t) \begin{pmatrix} w(0) \\ z(0) \end{pmatrix} \tag{3.10}$$

From (3.9) one easily proves that

$$\frac{d}{dt} \det R(t) = \operatorname{Tr} A(t) \det R(t)$$

The form (3.8) of $A(t)$ then gives

$$\det R(t) = e^{-2k^2 t} \tag{3.11}$$

Since $A(t)$ is periodic with period $T(P)$, the theorem of Floquet states that the matricant $R(t)$ can be written as

$$R(t) = Q(t)\,e^{Ct} \tag{3.12}$$

in which C is a constant matrix and $Q(t)$ is periodic with period T and $Q(0) = Q(T) = I$. Equations (3.7) are stable for $t \to +\infty$ iff all eigenvalues of $R(T) = e^{CT}$ lie on or within the unit circle.

This $R(T)$ can be constructed by calculating the change during one period of two specially chosen initial perturbations

$$\chi_1(0)=\begin{pmatrix} w_1(0) \\ z_1(0) \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi_2(0)=\begin{pmatrix} w_2(0) \\ z_2(0) \end{pmatrix}=\begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.13}$$

where we have put $t=0$ at the point where $\chi_1(0)$ is tangential to the orbit and $\chi_2(0)$ perpendicular to it. The matricant at time T then becomes

$$R(T)=\begin{pmatrix} w_1(T) & w_2(T) \\ z_1(T) & z_2(T) \end{pmatrix} \tag{3.14}$$

Since $\chi_1(t)$ will be tangent to the orbit, not only at $t=0$, but for all times, we find that $\chi_1(T)=\chi_1(0)$, so $w_1(T)=1$ and $z_1(T)=0$. If this is substituted into (3.11) we find $z_2(T)=e^{-2k^2T}$ and $R(T)$ takes the form

$$R(T)=\begin{pmatrix} 1 & w_2(T) \\ 0 & e^{-2k^2T} \end{pmatrix} \tag{3.15}$$

The eigenvalues are

$$\lambda_+=1 \quad \text{and} \quad \lambda_-=e^{-2k^2T} \tag{3.16}$$

which for all k lie on or inside the unit circle. The uniform and periodic solutions of (3.2) are therefore (marginally) stable.

Uniform solutions for which one species is extinct can also be found. Taking, e.g. $C=0$, which corresponds to $y=-1/3$, Eq. (3.2) reduces to:

$$\frac{dx}{dt}=\frac{1}{2}\sqrt{3}\left(x^2-\frac{1}{3}\right) \tag{3.17}$$

which has the solution

$$x(t)=-\frac{1}{\sqrt{3}}\tanh\left(\frac{1}{2}t\right) \tag{3.18}$$

The stability equations (3.7) for this solution become

$$\frac{dw}{dt}=-\left[k^2+\tanh\left(\frac{1}{2}t\right)\right]w+\frac{2}{\sqrt{3}}z \tag{3.19}$$

$$\frac{dz}{dt}=\left[-k^2+\tanh\left(\frac{1}{2}t\right)\right]z \tag{3.20}$$

For a perturbation $z(0)=0$ along the line $y=-1/3$, Eq. (3.20) is satisfied by $z(t)\equiv 0$, and (3.19) then shows that $w(t)\to 0$ for $t\to\infty$, so that the motion is stable. If, however, $z(0)\neq 0$, we see from (3.20) that for $k^2<1$ the function $z(t)$ eventually will increase. Therefore the solution (3.18) is not stable.

3.2. Nonuniform Solutions

We will now look for nonuniform solutions, in particular for the case that one of the species A, B, or C is nearly extinct. First consider the case that, say, C is completely extinct. In the x, y coordinates this corresponds to $y\equiv -1/3$. The equation for x then reduces to

$$\frac{\partial^2 x(u,t)}{\partial u^2}=\frac{\partial x}{\partial t}-\frac{1}{2}\sqrt{3}\left(x^2-\frac{1}{3}\right) \tag{3.21}$$

As was mentioned in the introduction, (3.21) is equivalent with the famous Fisher–Kolmogorov equation. Of particular interest are traveling wave solutions of the form

$$x(u,t)=v(u-ct)=v(z) \tag{3.22}$$

Substituting (3.22) into Eq. (3.21) yield

$$v''+cv'+\tfrac{1}{2}\sqrt{3}\,(v^2-\tfrac{1}{3})=0 \tag{3.23}$$

where differentiation is with respect to z. Written as a system, this becomes

$$\begin{aligned} v_1' &= v_2 \\ v_2' &= -cv_2-\tfrac{1}{2}\sqrt{3}\,(v_1^2-\tfrac{1}{3}) \end{aligned} \tag{3.24}$$

Equation (3.24) has an unstable fixed point at $(v_1, v_2)=(-1/\sqrt{3}, 0)$ and a stable fixed point at $(v_1, v_2)=(1/\sqrt{3}, 0)$.

For $c=2$ there exists a heteroclinic connection between these fixed points, which for $\tau\to -\infty$ approaches $(-1/\sqrt{3}, 0)$ via the unstable eigenvector and for $\tau\to\infty$ approaches $(1/\sqrt{3}, 0)$ via the unique eigenvector at that point. [The value $c=2$ is special, because Eq. (3.24), when linearized in $(1/\sqrt{3}, 0)$, has two equal negative eigenvalues, but only one eigenvector.]

This heteroclinic connection corresponds to a moving front solution of (3.21) traveling with a speed $c=2$.

Although (3.24) admits heteroclinic solutions for all $c \geq 2$, the value $c=2$ is particularly relevant, because it was shown by many authors (beginning with Kolmogorov in 1937) that a wide variety of initial conditions will all eventually develop into a moving front solution with $c=2$. For details and references see section 11.3 in Ref. 3.

Motivated by these results, we now look for solutions of (3.1) of the form

$$x(u, t) = v(u-ct) = v(z), \qquad y(u, t) = w(u-ct) = w(z) \tag{3.25}$$

with $c=2$ and assuming that y is near $y=-1/3$. Substituting (3.25) into (3.1) yields the system

$$\begin{aligned} v_1' &= v_2 \\ v_2' &= -cv_2 - \tfrac{1}{2}\sqrt{3}\,(\tfrac{2}{3}w_1 + v_1^2 - w_1^2) \\ w_1' &= w_2 \\ w_2' &= -cw_2 + \sqrt{3}\,(\tfrac{1}{3}v_1 + v_1 w_1) \end{aligned} \tag{3.26}$$

where again differentiation is with respect to z. Obviously, the plane $w_1 = -1/3$, $w_2 = 0$ is invariant, corresponding to the extinction of species C. By symmetry, there exist similar invariant planes corresponding to the extinction of A and B. respectively. Within each invariant plane the phase diagram of (3.26) looks the same as that of (3.24). Apart from $(v, w) = 0$, there exist three fixed points, corresponding to the extinction of two of the three species. Each of these fixed points lies in two invariant planes and we can construct a heteroclinic cycle between these points. Starting in $(v_1, v_2, w_1, w_2) = (-1/\sqrt{3}, 0, -1/2, 0)$ (this point corresponds to the situation that $B=C=0$), there exists a heteroclinic connection to $(v_1, v_2, w_1, w_2) = (1/\sqrt{3}, 0, -1/3, 0)$ (corresponding to $A=C=0$), lying in the plane $C=0$. By symmetry there exists a connection between this point and $(v_1, v_2, w_1, w_2) = (0, 0, 2/3, 0)$ (corresponding with $A=B=0$) and back to $(-1/\sqrt{3}, 0, -1/3, 0)$.

Numerical simulations have shown that this cycle is attracting. When we start near one of the fixed points (say $B=C=0$), the solution will closely follow the heteroclinic solution in the invariant plane $C=0$, eventually coming close to the fixed point $A=C=0$. After some time, the solution will then follow the heteroclinic connection in the $A=0$ plane, eventually coming close to the point $A=B=0$, and so on in a cyclical fashion. We have found numerically that after each cycle, the minimal distance to the fixed point has decreased. In fact, this series of minimal distances converges very rapidly to zero. Correspondingly, the "time" spent near a fixed point grows with every cycle.

This solution has the following interpretation. An observer at a fixed point u on the line will first observe that B is approximately 1, and A and C approximately 0. After some time, this observer will see a front of species A pass, moving with speed $c = 2$, and for a long time A will remain approximately 1 and B and C approximately 0. Some time later still, a front of species C will pass, and so on. The times between two successive fronts passing will grow ever larger, and after each cycle, the value of B will be closer to 1 (and A and C closer to 0).

In the case of the Fisher–Kolmogorov equation there exists one particular solution (the heteroclinic connection when $c = 2$), which can be shown to be stable under small perturbations with certain regularity conditions, for instance, exponential decay at $\pm\infty$. (For exact formulations we refer to Ref. 8). In the present case, there exists a whole family of solutions, characterized by the cyclical behavior sketched above. Although we have no proof, we believe that this family is stable, in the sense that a small, regular perturbation of a solution in this family will eventually converge to another member of this family.

4. ADDING THE REVERSE REACTION (R) ($\alpha > 0$)

For $\alpha > 0$, the equations for solutions which are uniform in space become

$$\begin{aligned} \frac{dx(t)}{dt} &= -f\frac{\partial P}{\partial y} + \alpha\frac{\partial V}{\partial x} \\ \frac{dy(t)}{dt} &= f\frac{\partial P}{\partial x} + \alpha\frac{\partial V}{\partial y} \end{aligned} \tag{4.1}$$

From (1.2)–(1.4) it follows that

$$\frac{1}{P(t)}\frac{dP(t)}{dt} = -\frac{9}{4}\alpha(x^2 + y^2) \tag{4.2}$$

so that $dP/dt < 0$. This means that the orbit is pushed against the sides of the triangle and none of the periodic solutions survives. In Fig. 4 some solutions of (4.1) are shown.

4.1. Ginzburg–Landau Approximation

In Section 2.1 it was shown that for $\alpha > 0$, the solution $x = y = 0$ (corresponding to $A = B = C = 1/3$) is unstable. We now want to study the behavior of solutions of (1.5) near this fixed point when $\alpha > 0$ but small.

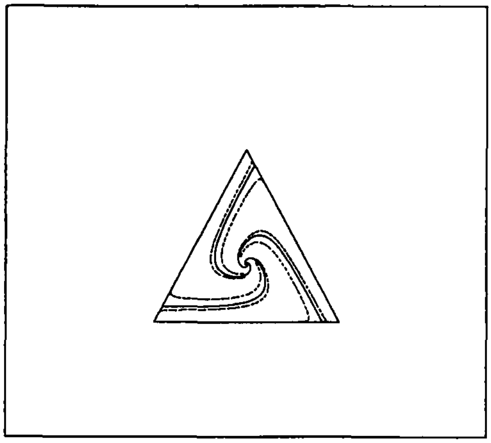

Fig. 4. Some solutions of (4.1).

The standard procedure in this case is to derive a Ginzburg–Landau equation.

The dispersion relation $\lambda_{\pm} = \alpha/6 - k^2 \pm (i/2) f(\alpha)$ of (2.2) leads to the instability curve $\mathrm{Re}(\lambda_{\pm}) = \alpha/6 - k^2 = 0$.

From this it follows that for $\alpha < 0$, all perturbations decay. At $\alpha = \alpha_c = 0$, perturbations with wavenumber $k = k_c = 0$ become unstable. When $\alpha > 0$ there is an interval, defined by $k^2 < \alpha/6$, of unstable wavenumbers. When $\alpha = \alpha_c$ and $k = k_c$, the solution of (3.1) is given in linear approximation by the so-called critical wave: $(x, y)^T = re^{i\omega_c t}(1, i)^T + \text{c.c.}$, where $\omega_c = 1/2f(0) = 1/\sqrt{3}$, r is small, and c.c. stands for complex conjugation.

In order to study the bifurcations of the solution $x = y = 0$ at $\alpha = \alpha_c$, we scale α by $\alpha = \varepsilon^2\tilde{\alpha}$ and substitute for $(x, y)^T$ an expansion in ε and Fourier modes, the first term of which is a slow modulation of the critical wave: $(x, y)^T = \varepsilon A(\xi, \tau)\, e^{i\omega_c t}(1, i)^T + \mathcal{O}(\varepsilon^2) + \text{c.c.}$

The variables ξ and τ are rescaled space and time coordinates: $\xi = \varepsilon u$, $\tau = \varepsilon^2 t$. Using a well-known procedure,[9] we can derive an equation for $A(\xi, \tau)$,

$$\frac{\partial A}{\partial \tau} = \frac{\partial^2 A}{\partial \xi^2} + \frac{\tilde{\alpha}}{6}(1 - i\sqrt{3})\, A + 2i\sqrt{3}\, A\, |A|^2 \tag{4.3}$$

Equation (4.3) is an instance of the Ginzburg–Landau equation. There exists a vast literature on this equation. However, (4.3) is rather exceptional since most authors study the Ginzburg–Landau equation under the assumption that the real part of the coefficient of the $A\,|A|^2$ term is negative. In this case it is zero, which makes (4.3) *degenerate*. In general there are doubts as to whether such an equation will be a valid approximation.[10] In spite of this we will use it, for reasons which will become clear in the following section.

Equation (4.3) admits solutions of the type $A(\xi, \tau) = \tilde{R}e^{i(k\xi + \omega\tau)}$. Substitution yields

$$\omega = -\frac{\tilde{\alpha}}{2\sqrt{3}} + 2\sqrt{3}\,\tilde{R}^2, \qquad k^2 = \frac{\tilde{\alpha}}{6} \tag{4.4}$$

In terms of the original variables, this solution becomes

$$\begin{pmatrix} x(u,t) \\ y(u,t) \end{pmatrix} = R \exp\left\{\frac{i}{\sqrt{3}}\left[\left(1 - \frac{\alpha}{2} + 6R^2\right)t - \sqrt{\frac{\alpha}{2}}\,u\right]\right\}\begin{pmatrix} 1 \\ i \end{pmatrix} + \text{c.c.} \tag{4.5}$$

where $R = \varepsilon\tilde{R}$.

4.2. Exact Solutions

It should be stressed that if (4.5) is a valid approximation at all, it is expected to be so only near $x = y = 0$ and for small values of $\alpha > 0$. It is remarkable, however, that a much better result can be obtained than expression (4.5). In fact, we can find exact solutions of (1.5) of roughly the same form as (4.5), and not necessarily near $x = y = 0$, for all values of $\alpha > 0$. There seems to be no structural reason for this phenomenon, which was a computer-assisted discovery.

Substituting into Eq. (1.5) the expressions (with some notational abuse)

$$x(u,t) = x(u - ct) = x(z), \qquad y(u,t) = y(u - ct) = y(z) \tag{4.6}$$

where the speed c is as yet undetermined, leads to the equations

$$\begin{aligned} \frac{d^2x}{dz^2} &= -c\frac{dx}{dz} + f(\alpha)\frac{\partial P}{\partial y} - \alpha\frac{\partial V}{\partial x} \\ \frac{d^2y}{dz^2} &= -c\frac{dy}{dz} - f(\alpha)\frac{\partial P}{\partial x} - \alpha\frac{\partial V}{\partial y} \end{aligned} \tag{4.7}$$

This is a four-dimensional system of ordinary differential equations, for which there is no *a priori* hope that something can be said about its solutions. However, numerical solutions suggested that for a particular value of c, namely

$$c = c_0 = \frac{|2-\alpha|}{\sqrt{2\alpha}} \tag{4.8}$$

all solutions tended to orbits for which $P(x, y) = \text{const}$. The value of c_0 was found by linearizing (4.7) near $x = y = 0$ and determining the value of c for which bounded solutions existed for $z \to \pm\infty$.

The numerical suggestion was confirmed when it was found that differentiating the expression

$$\begin{aligned} \frac{dx}{dz} &= \frac{f(\alpha)}{c_0} \frac{\partial P}{\partial y} \\ \frac{dy}{dz} &= -\frac{f(\alpha)}{c_0} \frac{\partial P}{\partial x} \end{aligned} \tag{4.9}$$

with respect to z leads to the relations

$$\begin{aligned} \frac{d^2x}{dz^2} &= -\alpha \frac{\partial V}{\partial x} \\ \frac{d^2y}{dz^2} &= -\alpha \frac{\partial V}{\partial y} \end{aligned} \tag{4.10}$$

From this it follows that a solution of (4.9) automatically satisfies (4.7), when $c = c_0$. A more geometrical picture of the situation is obtained by writing (4.7) as a system

$$\begin{aligned} x_1' &= x_2 \\ x_2' &= -cx_2 + f(\alpha) \frac{\partial P(x_1, y_1)}{\partial y_1} - \alpha \frac{\partial V(x_1, y_1)}{\partial x_1} \\ y_1' &= y_2 \\ y_2' &= -cy_2 - f(\alpha) \frac{\partial P(x_1, y_1)}{\partial x_1} - \alpha \frac{\partial V(x_1, y_1)}{\partial y_1} \end{aligned} \tag{4.11}$$

where we consider $\alpha > 0$ a fixed constant, c a bifurcation parameter, and differentiation is with respect to z. When $c = c_0$, the solution $(x_1, x_2, y_1, y_2) = (0, 0, 0, 0)$ undergoes a Hopf bifurcation, or at least the linearization of

(4.11) in this point has two purely imaginary eigenvalues and two eigenvalues with negative real parts. According to centre-manifold theory,[11] there then exists an invariant, locally attracting two-dimensional manifold. In this case, from (4.9) we derive an explicit parametrization of this manifold:

$$\begin{aligned} x_2 &= \frac{f(\alpha)}{c_0} \frac{\partial P(x_1, y_1)}{\partial y_1} \\ y_2 &= -\frac{f(\alpha)}{c_0} \frac{\partial P(x_1, y_1)}{\partial x_1} \end{aligned} \tag{4.12}$$

The flow on this manifold is given by (4.9), which admits a constant of motion, namely $P(x_1, y_1) = \text{const}$. This implies that the Hopf bifurcation is degenerate.

Equations (4.9) are very similar to the uniform equations (3.2). In fact, after scaling z by $\tilde{z} = -[f(\alpha)\sqrt{3}/2c_0]\, z$, Eqs. (4.9) will have exactly the same form as (3.2), but now with $\tilde{z}$ instead of t as the independent variable.

The solutions of (3.2) are periodic and the orbits are fully determined by the value of $P(x, y)$. Let $P(x, y) = p$ and denote the solution of (3.2) by $(x_p(t), y_p(t))$. Then the solution of (4.9), which is also a solution of (4.11), is $(x_p(\tilde{z}), y_p(\tilde{z}))$. Solutions of this form can be described as *traveling periodic waves*. In terms of the original variables, we find

$$x(u, t) = x_p\left(\left(1 - \frac{1}{2}\alpha\right)t - \sqrt{\frac{\alpha}{2}}\,u\right), \qquad y(u, t) = y_p\left(\left(1 - \frac{1}{2}\alpha\right)t - \sqrt{\frac{\alpha}{2}}\,u\right) \tag{4.13}$$

For $p \approx 1/27$, x_p and y_p are near $x = y = 0$ and the linear approximation is given by

$$(x_p(\tilde{z}), y_p(\tilde{z}))^T \approx R \exp\left(\frac{i}{\sqrt{3}}\tilde{z}\right)(1, i)^T + \text{c.c}$$

with R small. Combining with (4.13) yields the approximation

$$(x(u, t), y(u, t))^T = R \exp\left[\frac{i}{\sqrt{3}}\left(\left(1 - \frac{\alpha}{2}\right)t - \sqrt{\frac{\alpha}{2}}\,u\right)\right](1, i)^T + \text{c.c} \tag{4.14}$$

Comparing (4.14) with (4.5), it is seen that (4.5) is a "nonlinear correction" on the linear approximation (4.14).

However, (4.5) is itself only an asymptotic solution, with a very limited range of validity.

The solution (4.13) is exact, valid for all $\alpha > 0$, and, because we can take any $0 < p < 1/27$, certainly not restricted to the neighborhood of $x = y = 0$—a remarkable result, since it is rare to find exact, nontrivial solutions of coupled nonlinear partial differential equations.

4.3. Stability

The question of stability of the solutions (4.13) leads to formidable analytic difficulties. We can, however, study the stability of these solutions when (x, y) are near $x = y = 0$, by using the Ginzburg–Landau equation (4.3) as an approximation.

Putting

$$A(\xi, \tau) = (R + \rho(\xi, \tau)) \exp i\{k\xi + \omega\tau + \theta(\xi, \tau)\} \tag{4.15}$$

substituting into (4.3), and using the relations (4.4) then leads to equations for $\rho(\xi, \tau)$ and $\theta(\xi, \tau)$. Linearizing these equations and substituting $(\rho(\xi, \tau), \theta(\xi, \tau))^T = e^{iq\tau}(X(\tau), Y(\tau))^T$ then yields a two-dimensional system of linear, ordinary differential equations:

$$\frac{d}{d\tau}\begin{pmatrix} X \\ Y \end{pmatrix} = L(q)\begin{pmatrix} X \\ Y \end{pmatrix} \tag{4.16}$$

where the linear operator $L(q)$ depends on the wavenumber q of the perturbation. The solution $A(\xi, \tau) = R \exp i\{k\xi + \omega\tau\}$ is stable iff the real part of the eigenvalues of $L(q)$ is nonpositive for all $q \in \mathbf{R}$. A tedious but straightforward calculation shows that this condition is not satisfied, and therefore these solutions are not stable.

As was noted earlier, the validity of (4.3) as an approximation of (1.5) is not established in full rigor. Because of the similarity of the solutions (4.14) and (4.5), however, we feel justified to conclude that "small solutions", i.e., solutions with $p \approx 1/27$, of type (4.13) are not stable. This method does not apply for other values of p, when the solution is not small. In those cases numerical studies (which we have not performed) may provide answers.

4.4. Behavior near the Boundary

When one of the species is extinct, say $C = 0$, the equations reduce to

$$\frac{\partial^2 x(u, t)}{\partial u^2} = \frac{\partial x}{\partial t} - \frac{1}{2}\sqrt{3}\left(x^2 - \frac{1}{3}\right) + \frac{\alpha}{2}\sqrt{3}\left(x^2 - \frac{1}{3}\right)\left(\frac{1}{2} + \frac{1}{2}\sqrt{3}\,x\right) \tag{4.17}$$

This equation closely resembles the one studied in Ref. 12. As in the case $\alpha = 0$, we can find traveling front solutions connecting the critical points which correspond to the situations $A = 1$, $B = 0$ and $A = 0$, $B = 1$, respectively. The minimum value of the speed c for which such solutions exist is $c_1(\alpha) = 2\sqrt{1-\alpha}$. Note that $c_1(0) = 2$, the value which was found in Section 3.

However, when we take $c = c_0 = (2-\alpha)/\sqrt{2\alpha}$, we can use the same method as in Section 4.2, and construct an explicit solution:

$$x(u, t) = \frac{1}{\sqrt{3}} \tanh \left\{ \frac{1}{4} \left[\sqrt{2\alpha}\, u - (2-\alpha)\, t \right] \right\}, \qquad y(u, t) = -\frac{1}{3} \tag{4.18}$$

In Fig. 5 the values of $c_0(\alpha)$ and $c_1(\alpha)$ are plotted.

Following an argument in Ref. 10, it can be shown that for $\alpha < 2/3$ a front will develop which travels with speed $c_1(\alpha)$. When $\alpha > 2/3$, the speed will be $c_0(\alpha)$.

When one of the species is *nearly* extinct, we expect the same behavior as in the $\alpha = 0$ case: a series of traveling fronts, with the distances between successive fronts growing increasingly larger. When α is small, the numerical results for the case $\alpha = 0$ can be used to show that this is the case, the speed of the fronts being $c_1(\alpha)$. For larger α, a separate numerical simulation should be made to confirm our hypothesis.

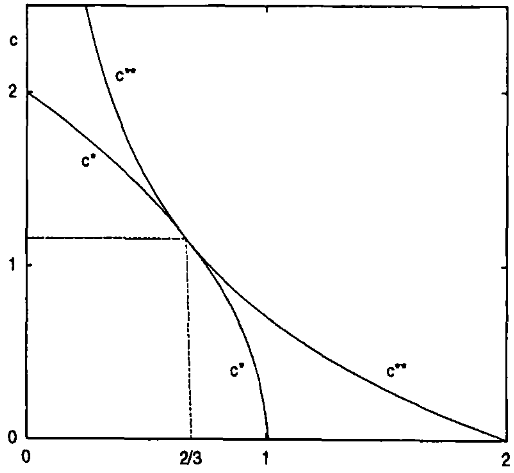

Fig. 5. Velocities $c^{**} = c_0(\alpha)$ and $c^* = c_1(\alpha)$ versus α.

5. CONCLUSIONS

In this paper we have studied the behavior of a reaction–diffusion system with three species A, B, and C on a line, which participate in the reactions

$$A+B\to 2A,\qquad B+C\to 2B,\qquad C+A\to 2C\quad (\mathrm{D})$$

and

$$A+2B\to 3B,\qquad B+2C\to 3C,\qquad C+2A\to 3A\quad (\mathrm{R})$$

The reaction (R) has a rate α with respect to the reaction (D). At a given time t and position u along the line, the concentrations A, B and C are represented by a point inside an equilateral triangle of unit height (see Fig. 1). we restrict ourselves to the case where the sum is and remains constant.

We will now describe what we understand about the behavior of this system and what are still open questions.

For that purpose we will distinguish four classes: First, there are the fixed points. The point M represents the situation where all species are in equilibrium. This point is stable when $\alpha<0$ and unstable when $\alpha>0$. The corner points represent situations where two of the three species are extinct. These points are unstable when $\alpha<1$ and become stable when $\alpha>1$. At $\alpha=1$ three new fixed points bifurcate from the corner points. They are unstable for $\alpha>1$.

Second, we have invariant subspaces, corresponding to the situation that one of the species is extinct. In this invariant subspace the problem reduces to the Fisher–Kolmogorov equation. Typically we find moving front solutions with speed $c=2\sqrt{1-\alpha}$ when $0\leqslant\alpha<2/3$ and $c=(2-\alpha)/\sqrt{2\alpha}$ when $2/3\leqslant\alpha<1$.

Third, we have a family of solutions for which none of the species is extinct. For $\alpha=0$ the equations for the uniform solution are Hamiltonian, leading to a family of periodic solutions $(x_p(t), y_p(t))$, parametrized by the value of $P(x, y)=p$. In a remarkable discovery, we have found that for $\alpha>0$ the system admits solutions of the form

$$\left(x_p\left(\left(1-\tfrac{1}{2}\alpha\right)t-\sqrt{\tfrac{1}{2}\alpha}\,u\right),\ y_p\left(\left(1-\tfrac{1}{2}\alpha\right)t-\sqrt{\tfrac{1}{2}\alpha}\,u\right)\right)$$

which can be called traveling periodic waves.

Finally, another family of solutions for which none of the species is extinct is given by a type of generalization of the Fisher–Kolmogorov fronts. These solutions consist of a series of successive fronts, where the times between two passing fronts grow increasingly larger.

The most important open problem concerns the stability of the solutions in the last two classes. We conjecture that, at least for α small, the successive front family is stable in some sense.

As to the stability of the traveling periodic waves when $\alpha > 0$, we simply have no idea. For $\alpha = 0$ these solutions correspond to the uniform solutions, which we have shown to be (marginally) stable.

Connected with these stability questions is the problem of the final state of a given initial distribution. For $\alpha = 0$ there are at least two stable types of eventual behavior: a uniform solution and a successive front solution. Predicting which one will prevail, or whether perhaps there is yet another possibility, is a very interesting, but open problem.

Most of the analytical methods which have been applied in the present paper will be of no use when the model is extended to two and three dimensions. Probably the best way to investigate the new phenomena which will undoubtedly appear is to construct a cellular automaton with the same general behavior. This undertaking we will leave, however, to Matthieu Ernst, to whom this article is dedicated on the occasion of his 60th birthday.

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