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Periodic Waves in Reaction-Diffusion Models of Oscillatory Biological Systems

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Abstract. Many systems in biology and chemistry have been successfully modelled by oscillatory reaction-diffusion equations. In such equations, periodic waves are a fundamental solution type, and have been extensively studied. In this paper, the author discusses ways in which periodic waves can arise naturally from simple initial conditions. The mechanisms by which a particular wave is selected by the details of the initial data are explained, and formation of periodic waves behind invasive transition fronts is discussed. In some cases, the selection mechanism can cause an unstable wave to form, in which case it degenerates into spatiotemporal irregularities. This process is described and numerical evidence is given which suggests that these irregularities are genuinely chaotic. The various results have applications to a number of real oscillatory systems, and applications to intracellular calcium signalling and predator-prey invasion are discussed in detail.

1. Oscillatory Systems

Many systems in biology and chemistry are intrinsically oscillatory. In such cases, the stable state in the absence of spatial variation is not a stationary equilibrium, but rather consists of temporal oscillations in the interacting chemical or biological species. Examples include intracellular calcium signalling, the Belousov-Zhabotinskii reaction and some predator-prey interactions. These systems also exhibit spatial interactions, which are often modelled by diffusion. This combination of local oscillations and spatial diffusion produces a very wide range of spatiotemporal behaviours, including spiral waves, target patterns and spatiotemporal chaos (reviewed by MURRAY, 1989, Chapter 12). In one spatial dimension, the equivalent of both spiral waves and target patterns are periodic travelling waves, which are periodic functions of space and time, moving with constant shape and speed. This paper is concerned with these periodic wave solutions. In this first section, I review old results on the form, possible speeds, and stability of periodic

waves. In Section 2, I discuss the way in which periodic waves can be induced by a wide range of initial conditions; this has specific applications to intracellular calcium signalling. In Section 3, I show that periodic waves also arise naturally behind invasive transition fronts, and I discuss the application to predator-prey interactions in ecology. Finally, in Section 4, I consider the way in which, in both these applications, the generation of unstable periodic waves can act as a natural route to spatiotemporal chaos.

Periodic travelling waves occur in any reaction-diffusion system with oscillatory kinetics, by which I mean that the kinetic ODEs contain a stable limit cycle. Throughout this paper I will restrict attention to systems of two coupled reaction-diffusion equations, with the form

$$\partial u / \partial t = D_u \partial^2 u / \partial x^2 + f_u(u,v) \tag{1a}$$

$$\partial v / \partial t = D_v \partial^2 v / \partial x^2 + f_v(u,v). \tag{1b}$$

Here $u(x,t)$ and $v(x,t)$ denote the concentrations or densities of the interacting species; x and t denote space and time, respectively, and D_u and D_v are positive constants. For this system, travelling waves are solutions with the form $u(x,t) = U(z)$ and $v(x,t) = V(z)$, where $z = x - at$ is the travelling wave coordinate and a is the wave speed. Such solutions satisfy

$$D_u U'' + aU' + f_u(U,V) = 0 \tag{2a}$$

$$D_v V'' + aV' + f_v(U,V) = 0, \tag{2b}$$

where prime denotes d/dz. A periodic wave corresponds to a limit cycle solution of these travelling wave ODEs. KOPELL and HOWARD (1973) showed that whenever the kinetics f_u, f_v are oscillatory, (2) has a one-parameter family of such limit cycle solutions, arising from a Hopf bifurcation. A quite different issue, however, is whether these periodic waves are stable as reaction-diffusion solutions. If they are unstable, they will of course never be seen in a real system. This stability question has been addressed by a number of authors (KOPELL and HOWARD, 1973; OTHMER, 1977; COPE, 1980; MAGINU, 1979, 1981) but all that is known for general kinetics is that sufficiently close to the Hopf bifurcation in (2), the periodic waves are unstable, while for $|c|$ sufficiently large, the waves are stable. Thus slow, low amplitude waves are unstable, while sufficiently fast waves are stable. The stability change between these two extremes can in some cases be quite complex, with alternating regions of stability and instability. The observation that very fast waves are stable is expected intuitively since as the wave speed increases towards infinity, the spatial wavelength does also, and the periodic wave approaches the (spatially homogeneous) limit cycle solution of the kinetics.

Much of the progress on periodic travelling waves has been obtained using the "λ-ω" class of reaction-diffusion systems. These are systems of the form (1), specifically

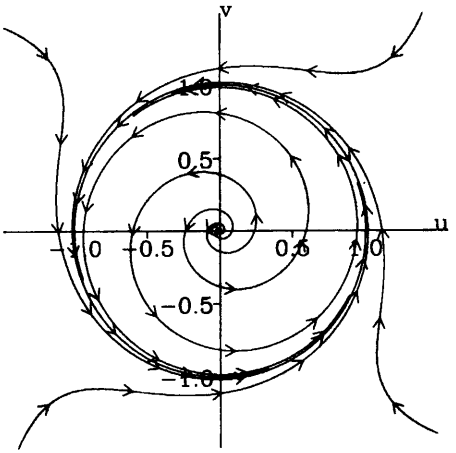

Fig. 1. An illustration of the phase plane for the kinetics of a λ-ω system in which $\lambda(.)$ is monotonically decreasing with $\lambda(r_0) = 0$, and $\omega(.)$ in either monotonically increasing or decreasing. There is a stable circular limit cycle of radius r_0. The particular phase plane illustrated is for $\lambda(r) = 1 - r^2$ and $\omega(r) = 3 - r^2$, so that $r_0 = 1$.

$$\partial u / \partial t = \partial^2 u / \partial x^2 + \lambda(r)u - \omega(r)v \tag{3a}$$

$$\partial v / \partial t = \partial^2 v / \partial x^2 + \omega(r)u + \lambda(r)v; \tag{3b}$$

here $r = (u^2 + v^2)^{1/2}$. For simplicity, I consider the case in which $\lambda(.)$ is monotonically decreasing with a simple zero at $r = r_0$, and $\omega(.)$ is either monotonically increasing or decreasing. Then the kinetic ODEs have a stable circular limit cycle of radius r_0 (Fig. 1). The beauty of λ-ω systems is that the family of periodic waves has a very simple analytical form, namely

$$u = \hat{r}\cos\left[\omega(\hat{r})t \pm \lambda(\hat{r})^{1/2}x\right] \tag{4a}$$

$$v = \hat{r}\sin\left[\omega(\hat{r})t \pm \lambda(\hat{r})^{1/2}x\right] \tag{4b}$$

(KOPELL and HOWARD, 1973; ERMENTROUT, 1980). Here $\hat{r} \in (0, r_0)$ parameterises the wave family. Moreover, an exact condition for the stability of (4) as a PDE solution was determined by KOPELL and HOWARD (1973), namely that

$$4\lambda(\hat{r})\left[1 + \left(\frac{\omega'(\hat{r})}{\lambda'(\hat{r})}\right)^2\right] + \hat{r}\lambda'(\hat{r}) \le 0 \tag{5}$$

must hold for linear stability. More recently, KAPITULA (1991) has investigated nonlinear stability.

2. Periodic Wave Evolution

Despite this considerable knowledge of the existence and properties of periodic waves, there was until very recently no work on the way in which periodic waves might arise in oscillatory systems. I will show that in both λ-ω and more general systems, a wide range of initial conditions do evolve quite naturally to periodic travelling waves. I will start by discussing the λ-ω case; more details on the calculations I discuss are given elsewhere (SHERRATT, 1993, 1994a). I consider the semi-infinite domain $0 < x < \infty$ with boundary conditions $\partial u/\partial x = \partial v/\partial x = 0$ at $x = 0$ and $u, v \to 0$ as $x \to \infty$. In an attempt to generate periodic waves, I consider initial data that decays exponentially in space:

$$u(x,0) = v(x,0) = Ae^{-\xi x}. \tag{6}$$

For a very wide range of functional forms for $\lambda(.)$ and $\omega(.)$, these initial conditions give rise to one particular member of the periodic wave family, occupying an expanding region of the spatial domain (Fig. 2). Thus the form of the solution is of a wave front moving across the domain, with periodic waves behind this front. The speed of the periodic waves is different from that of the advancing wave front, and in some cases they move in the opposite direction.

Numerical experimentation shows clearly that the speeds of both the advancing front and the periodic waves depend on the decay rate ξ of the initial data, but are independent of other details, such as the parameter A and the boundary conditions at $x = 0$. This dependence is most easily studied by working not in terms of the variables u and v, but rather in terms of polar coordinates r and θ in the u-v plane. Thus $r = (u^2 + v^2)^{1/2}$ as above, and $\theta = \tan^{-1}(v/u)$. Use of these variables is standard procedure when studying λ-ω systems, and the transformed partial differential equation is

$$r_t = r\lambda(r) + r_{xx} - r\theta_x^2 \tag{7a}$$

$$\theta_t = \omega(r) + \theta_{xx} + 2r_x\theta_x / r. \tag{7b}$$

When the numerical solutions described above are plotted in terms of r and θ, they have a rather simple form, namely simple transition wave fronts in r and $\partial\theta/\partial x$ (Fig. 2). Ahead of the transition front, r and $\partial\theta/\partial x$ tend to zero, corresponding to $u = v = 0$, while behind the front, r and $\partial\theta/\partial x$ approach constant, non-zero values. From (4) it is clear that constant r and $\partial\theta/\partial x$ corresponds to periodic waves in u and v.

Based on these numerical observations, I look for a solution of (7) of the form $r = \tilde{r}(x - st)$, $\psi \equiv \theta_x = \tilde{\psi}(x - st)$, where s is the speed of the transition front. This implies that

$\theta(x,t) = \tilde{\Psi}(x-st)+f(t)$, where $\tilde{\Psi}(.)$ is an indefinite integral of $\tilde{\psi}(.)$, and $f(.)$ is an arbitrary function. As $x \to \infty$, $\tilde{r} \to 0$ and $\tilde{\psi} \to 0$, and thus substituting this solution form into (7b) and letting $x \to \infty$ implies that $f'(t) = \omega(0)$. Therefore I have the travelling front solution

$$r = \tilde{r}(x-st)$$

$$\theta = \tilde{\Psi}(x-st)+\omega(0)t+\theta_0$$

where θ_0 is an arbitrary constant.

Substituting this solution form into (7) gives a third order system of ordinary differential equations:

$$\tilde{r}''+s\tilde{r}'+\tilde{r}\lambda(\tilde{r})-\tilde{r}\psi^2 = 0 \tag{8a}$$

$$\tilde{\psi}'+(s+2\tilde{r}'/\tilde{r})\tilde{\psi}+\omega(\tilde{r})-\omega(0) = 0 \tag{8b}$$

where prime denotes d/dz. The steady states $r = r_s$, $\psi = \psi_s$ of (8) must satisfy $s\psi_s = \omega(0) - \omega(r_s)$ and $r_s[\lambda(r_s) - \psi_s^2] = 0$, so that either $r_s = \psi_s = 0$ or

$$\left[\omega(0)-\omega(r_s)\right]^2 = s^2\lambda(r_s). \tag{9}$$

The first of these is the steady state ahead of the r-ψ transition front, and the second is an equation for the amplitude $\hat{r}$ of the periodic plane waves behind this front. My monotonicity assumptions for $\lambda(.)$ and $\omega(.)$ ensure that this equation will have a unique solution for any given value of s.

The value of s remains to be determined, however. In scalar reaction-diffusion equations such as the Fisher equation (FISHER, 1937; KOLMOGOROV *et al.*, 1937; ROTHE, 1978), it is known that the speed of a wave front is determined by the linearisation of the PDE ahead of the front. With this in mind, I linearise (7) about $r = 0$, giving

$$\partial r/\partial t = \partial^2 r/\partial x^2 + \lambda(0)r.$$

This is identical to the linearisation of the Fisher equation

$$\partial y/\partial t = \partial^2 y/\partial x^2 + \lambda(0)y(1-y) \tag{10}$$

about $y = 0$, suggesting that the dependence of wave speed on initial data might be the same in the two cases. For (10), it was shown by ROTHE (1978) that if $y(x,0)$ is monotonically

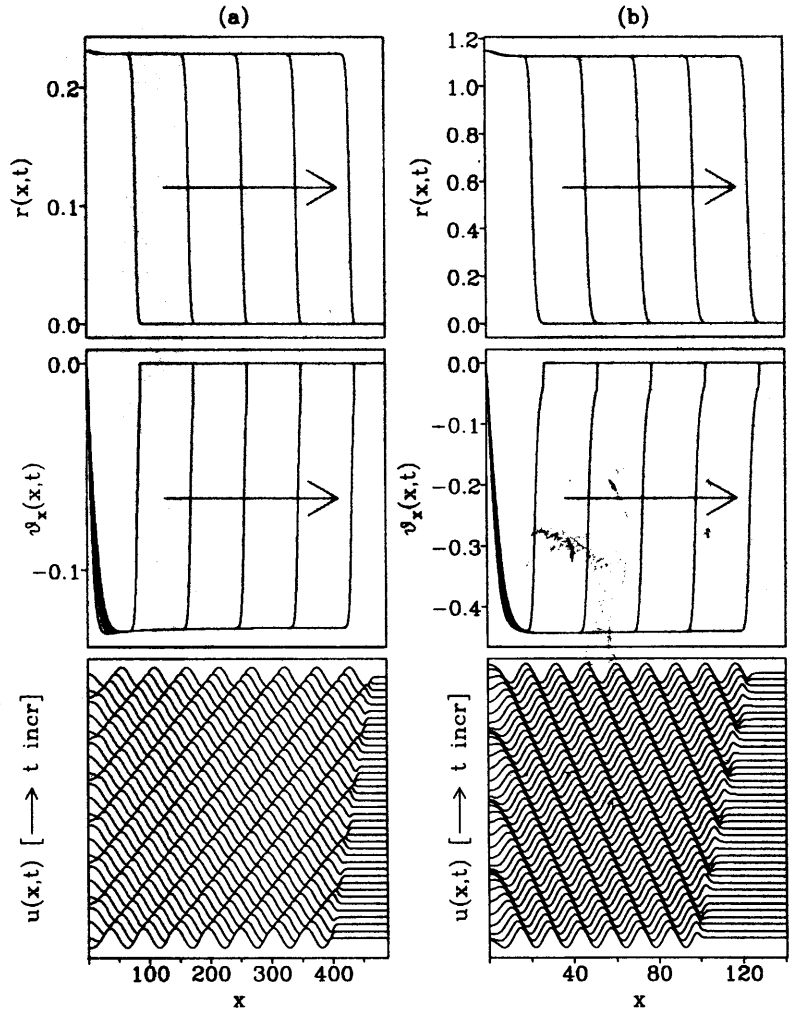

Fig. 2. Examples of the solution of (3) subject to (6) for monotonic $\lambda(.)$ and $\omega(.)$. I plot r and θ_x as functions of x at equally spaced times, and u as a function of x at successive times t, with the vertical spacing of solutions proportional to the time interval. In all cases, the solution evolves to transition fronts in r and θ_x, moving with constant shape and speed; the steady state behind the front corresponds to periodic plane waves. The sign of θ_x behind the front is positive or negative according to whether $\omega(.)$ is decreasing or increasing, respectively, and the direction of motion of the periodic plane waves is in the positive or negative direction according to whether $\omega(0)/\omega(\hat{r}) - 1$ is positive or negative, respectively. The functional forms for $\lambda(.)$ and $\omega(.)$ are: (a) $\lambda(r) = 2 - e^{3r}$, $\omega(r) = e^r$, with $\xi = 4$; (b) $\lambda(r) = 2 - r^5$, $\omega(r) = 4 - r^2$, with $\xi = 3$; (c) $\lambda(r) = (4 - r^6e^{2r})/\log(3 + r)$, $\omega(r) = 1 - r^4e^r$, with $\xi = 2$; (d) $\lambda(r) = 1 - 2\tanh r$, $\omega(r) = \log(2 + r)$, with $\xi = 4$. The time intervals between successive solutions for r and θ_x solutions are approximately (a) 44; (b) 8.9; (c) 6.4; (d) 47, and the range of times in the plots of $u(x,t)$ are (a) $187 \le t \le 220$; (b) $35.6 \le t \le 44.5$; (c) $6.4 \le t \le 32$; (d) $188 \le t \le 235$. The value of A was 0.1, but in fact the solutions are essentially independent of A. Here and in numerical solutions of the reaction-diffusion equations presented in other figures, the equations were solved using the method of lines and Gear's method.

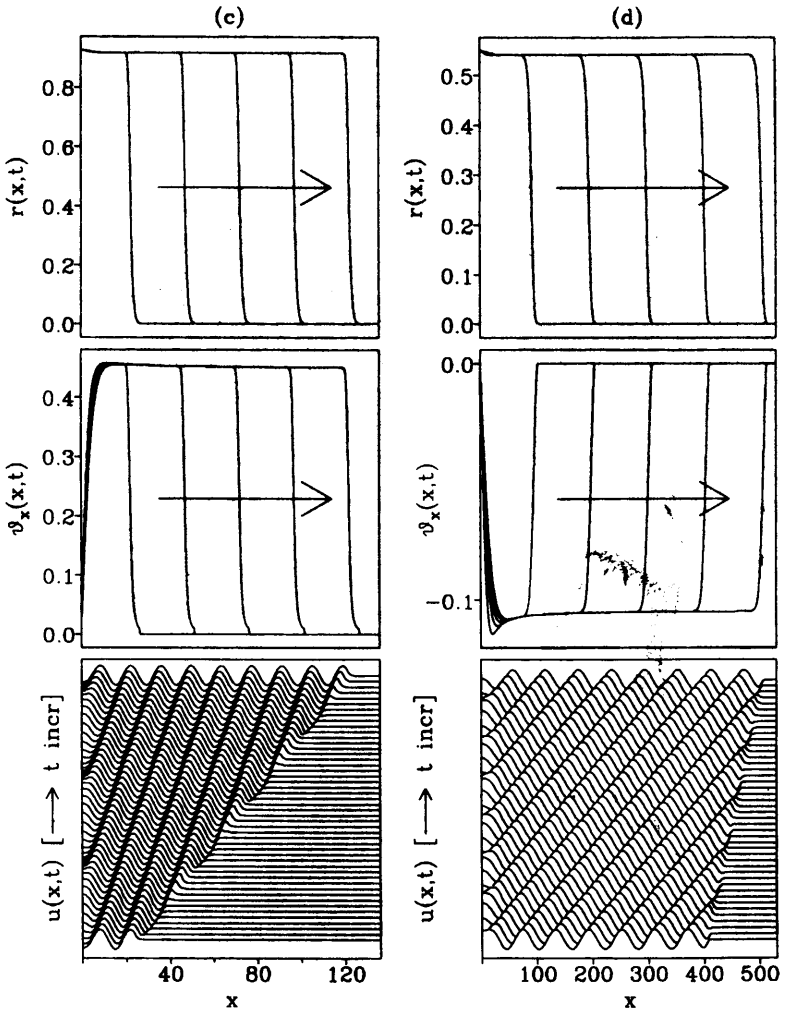

Fig. 2. (continued).

decreasing, with $y(x,0) \to 1$ as $x \to -\infty$ and $y(x,0) = \mathcal{O}_s(e^{-\xi x})$ as $x \to +\infty$, then the solution evolves to travelling wave fronts with speed

$$s = \begin{cases} \xi + \lambda_0 / \xi, & 0 < \xi \le \sqrt{\lambda_0} \\ 2\sqrt{\lambda_0}, & \xi \ge \sqrt{\lambda_0}. \end{cases} \tag{11}$$

This formula compares extremely well with the speeds of the $r - \partial\theta/\partial x$ transition front in numerical solutions of λ-ω systems. Thus the periodic wave generated by the initial data

(6) is related to the decay rate ξ by the combination of formulae (9) and (11).

In exactly the same way, exponentially decaying initial conditions generate periodic waves in a wide range of oscillatory reaction-diffusion systems (SHERRATT, 1994b). Here, the decay is of course to the steady state from which the kinetics limit cycle has bifurcated; typically this is a non-trivial steady state. The great advantage of the λ-ω case is the ability to study this generation analytically as just described; more generally I have been unable to make any analytic progress, and have to rely on numerical solutions alone. However, for a wide range of systems, these numerical results indicate a strong analogy with the λ-ω case, with the particular periodic wave that is selected being related to the initial decay rate via the transition front speed.

One particular situation in which this generation of periodic waves has specific application is intracellular calcium signalling. Calcium is an important intracellular second messager, and exhibits a wide range of spatial and temporal oscillations in response to different extracellular signals (BERRIDGE, 1990; TSIEN and TSIEN, 1990; SANDERSON *et al.*, 1990). A number of mathematical models have been proposed for calcium oscillations and waves in a variety of different cell types (GOLDBETER *et al.*, 1990; STUCKI and SOMOGYI, 1994; SNEYD *et al.*, 1995), and here I will discuss only the model of ATRI *et al.* (1993), which applies to the *Xenopus* oocyte. This model is based on the release of calcium from intracellular stores through channels that are sensitive to the regulatory molecule IP_3. External stimuli produce increased concentrations of IP_3, which causes the release of calcium from these internal stores. This cytosolic calcium then regulates further calcium release, with high calcium concentrations tending to inactivate the IP_3 receptors. Cytosolic calcium can itself be resequestered into the internal pool. The model of ATRI *et al.* (1993) models this process by two differential equations, with variables $c(x,t)$ and $n(x,t)$, denoting respectively the local calcium concentration and the fraction of receptors that have not been inactivated by calcium. The receptors are assumed to be stationary in space, so that the spatial variation is due entirely to the diffusion of calcium. The model equations are

$$\partial c/\partial t = \overbrace{D_c\partial^2 c/\partial x^2}^{\text{Diffusion}} + \overbrace{k_{\text{flux}}\mu n[b + (1-b)/(k_1 + c)]}^{\text{Calcium flux through IP}_3\text{ sensitive channels}} - \overbrace{\gamma c/(k_\gamma + c)}^{\text{Calcium-regulated pumping of calcium out of cytosol}} \quad (12a)$$

$$\tau_n \partial n/\partial t = \underbrace{k_2^2/(k_2^2 + c^2)}_{\text{Net production of new receptors}} - \underbrace{n.}_{\text{Receptor turnover}} \quad (12b)$$

Here the parameter μ is related to the IP_3 concentration. Depending on the value of this parameter, the model can be either excitable or oscillatory. In the oscillatory regime, with realistic values of the other parameters (ATRI *et al.*, 1993; SNEYD and SHERRATT, 1995), the calcium signalling waves have a form that is qualitatively very similar to Fig. 2(b). There is a leading wave front, moving with a speed of about 2 μm s^{-1}, and leaving periodic

waves in it wake. These periodic waves move in the opposite direction to the front, with a speed of about 30 μm s^{-1}.

One of a number of controversies on the propagation of calcium waves is whether the system is excitable or oscillatory in different situations; a detailed understanding of wave propagation in the oscillatory regime is an important step in this understanding. In practice, the waves travel through a medium that is not spatially uniform, due to unequal spacing of receptors, and the effects of this on oscillatory wave propagation are discussed elsewhere (SNEYD and SHERRATT, 1995).

3. Periodic Waves behind Invasion

Any oscillatory system will have an (unstable) steady state from which the kinetics limit cycle, and the periodic travelling waves, have bifurcated. However, in many cases there will also be other steady states, and this introduces a wide range of new wave behaviour. To be specific, I will focus on the particular case of predator-prey interactions, for which a number of different models have been proposed, with the form

$$\partial p / \partial t = D_p \partial^2 p / \partial x^2 + f_p(p,h) \tag{13a}$$

$$\partial h / \partial t = D_h \partial^2 h / \partial x^2 + f_h(p,h). \tag{13b}$$

Here $p(x,t)$ and $h(x,t)$ are the population densities of predators and prey, respectively, with diffusion coefficients D_p and D_h representing the motility of the populations. Biologically realistic models will have two non-trivial steady states, a "prey-only" state in which $p = 0$, $h = h_0$, and a "coexistence state", in which $p = p_s$, $h = h_s$, say. Intuitively one expects the prey-only state to be unstable to the introduction of predators, and in some cases the coexistence state is also unstable, with a stable limit cycle in the kinetics (Fig. 3). In such cases, the stable state in the absence of spatial variation is periodic temporal oscillations in prey and predator densities.

Systems of the form (13) have been used to study two main aspects of predator-prey dynamics: the formation of stationary spatial patterns (SEGEL and JACKSON, 1972; CONWAY, 1984; BENSON *et al.*, 1993) and the invasion of prey by predators (MURRAY, 1975; DUNBAR, 1983; HOLMES *et al.*, 1994). Here I am concerned with the latter application. Consider first a system for which the coexistence steady state is stable. Then there is a well-known travelling wave front solution of (13), which corresponds to invasion. Ahead of the front the system is in the prey-only state, with the coexistence state behind the front. This wave front is of course a heteroclinic connection between these two steady states in the travelling wave ODEs

$$D_p P'' + aP' + f_p(P,H) = 0 \tag{14a}$$

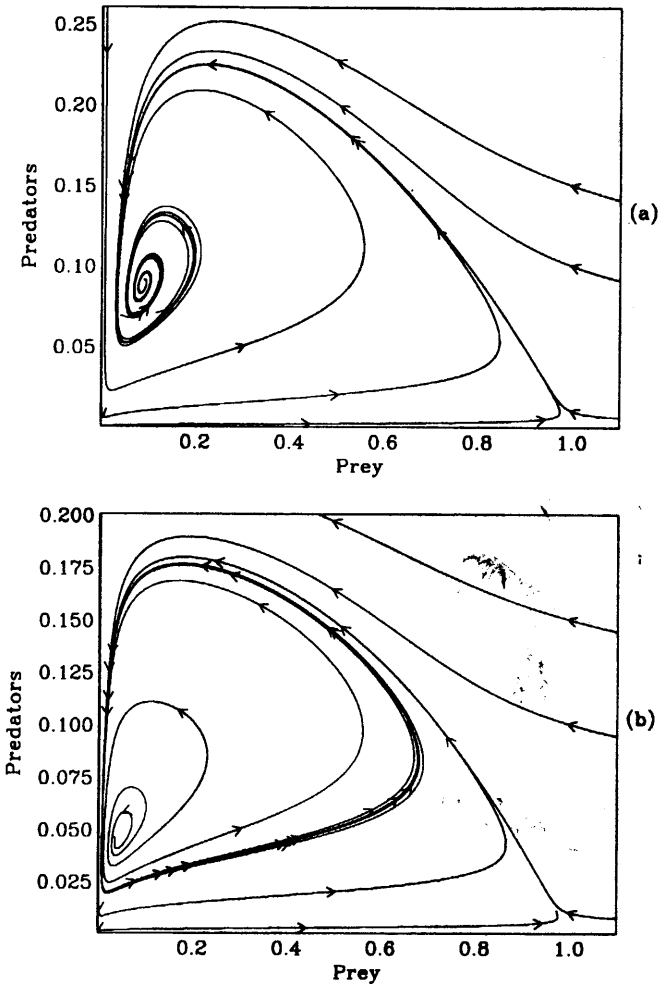

Fig. 3. Typical phase portraits of the population kinetics for a predator-prey system. There is a prey-only steady state (1,0) and also a coexistence steady state. In (a) the coexistence steady state in stable and the system is not oscillatory, while in (b) the system is oscillatory and the long-term behaviour is periodic oscillations in prey and predator densities, corresponding to the limit cycle in the phase plane. The actual phase planes shown are for $f_p(p,h) = B_p(1 - p/h)$, $f_h(p,h) = h(1 - h) - Ahp/(h + C)$ which is a standard predator-prey model (MURRAY, 1989). The parameter values are: (a) $A = 3$, $B = 0.3$ and $C = 0.2$; (b) $A = 3$, $B = 0.2$ and $C = 0.1$.

$$D_h H'' + aH' + f_h(P,H) = 0. \tag{14b}$$

Here $p(x,t) = P(z)$ and $h(x,t) = H(z)$ are travelling wave solutions; $z = x - at$ is the travelling wave coordinate and prime denotes d/dz. The parameter a is the speed of invasion; standard linear analysis about the leading edge of the wave shows that the speed of

invasion must be greater than or equal to $2\left[D_p\left(\partial f_p / \partial p\right)\big|_{p=0,h=h_0}\right]^{1/2}$, and numerical evidence suggests that for initial conditions corresponding to a spatially localised introduction of predators, the resultant invasive waves always travel at this minimum speed. In a four-dimensional system such as (14) it is notoriously difficult to prove the existence of a heteroclinic connection, but DUNBAR (1984) has actually done this for certain predator-prey models of the form (13).

When $p = p_s$, $h = h_s$ is unstable, so that the stable state in the kinetics is a limit cycle, the analogue of these invasive waves had not been considered until very recently. Figures 4(a) and (b) illustrate the numerical simulation of invasion in two such cases; the specific kinetic terms f_h and f_p are taken from a standard predator-prey model and are detailed in the figure legend. The initial conditions for these simulations are that the system is in the prey-only steady state everywhere except in a small localised region of space, in which predators are introduced. As in the non-oscillatory case, an invasive front moves out from the site of the initial perturbation; however the behaviour behind the front is quite new, consisting of spatiotemporal oscillations in both predator and prey densities. These oscillations appear to have the form of periodic travelling waves, and this is confirmed by detailed numerical tests (SHERRATT *et al.*, 1995a). For some parameter values, the periodic waves move in the same direction as the invading front, but with a faster speed (Fig. 4(a)), while for other parameters they move away from the invasive front (Fig. 4(b)).

This observation of periodic waves behind invasion was initially rather surprising, but in fact there is a simple explanation in the light of the discussion in Section 2. I have shown that initial conditions which decay exponentially to a limit cycle-related steady state evolve to periodic travelling waves, whose speed depends on the initial decay rate. In Section 2 I had in mind imposing these decaying initial conditions externally, but in the case of predator-prey invasion, an exponential decay arises quite naturally.

To see this, consider a particular model of form (13), and a parameter set for which the coexistence steady state is stable. Then the travelling wave ODEs (14) have a heteroclinic connection between the coexistence and prey-only steady states, which corresponds to the invasive wave solution of (13). Suppose now that a parameter in the kinetics is gradually altered, such that at some point the coexistence steady state undergoes a Hopf bifurcation, and the system becomes oscillatory. Despite this bifurcation, there is no change in the signs or characters of the eigenvalues at the coexistence steady state in the travelling front equations (14), and numerical continuation studies suggest that the heteroclinic connection continues to exist. Thus, even though the reaction-diffusion system (13) has become oscillatory, there continues to be an invasive travelling wave front solution, moving with the invasion speed a. However, the Hopf bifurcation in the kinetics does have a profound effect, causing this invasive wave front to become unstable as a PDE solution. This is clearly the case, since the coexistence state behind the invasive front is no longer stable.

The heteroclinic connection corresponding to the travelling front approaches the coexistence steady state along an eigenvector of the ODE system (14). This approach will thus be exponential in the travelling wave coordinate z. This implies that *the invasive*

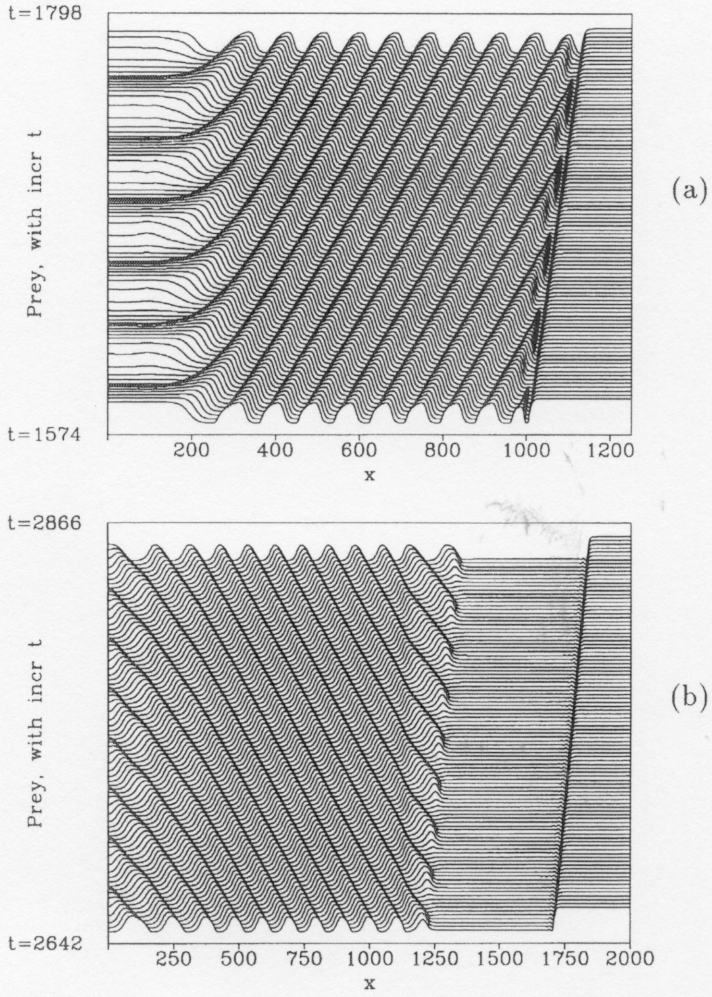

Fig. 4. An illustration of oscillatory wakes behind invasion in reaction-diffusion models of predator-prey interactions. The solutions I plot are for the system (13) with kinetics as in Fig. 3. The parameter values are: (a) $A = 3$, $B = 0.1$, $C = 0.1$; (b) $A = 3$, $B = 0.1$, $C = 0.2$. I plot prey density as a function of space at successive times, with the vertical separation of solutions proportional to the time interval. The form of the corresponding solutions for predator density is qualitatively very similar.

travelling wave front decays exponentially to the coexistence steady state behind the front. In the light of the discussion in Section 2, it seems possible that it is this exponential decay that induces the periodic waves seen in Fig. 4. I have used a simple numerical procedure to test this hypothesis. The first step in this is to calculate the eigenvalues and eigenvectors at the coexistence steady state in (14), from which the form of the approach to the steady state can be determined. In all cases I have considered, there are two complex conjugate

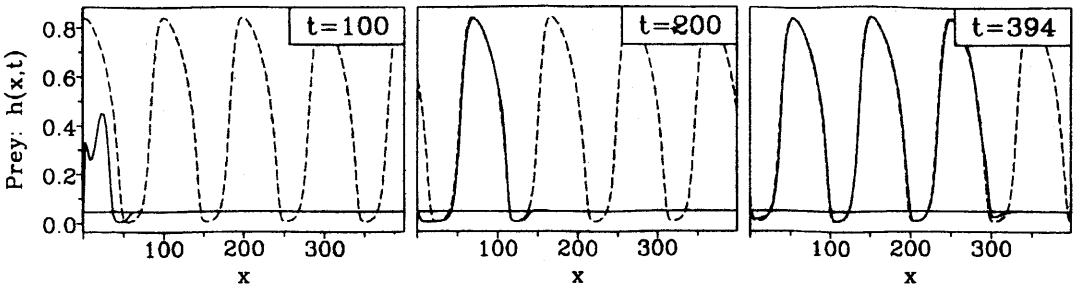

Fig. 5. The evolution of the solution of (13) following a small, exponentially decaying perturbation to the (unstable) coexistence steady state (p_s,h_s). The form of the perturbation has exactly the form of the tail of the invasive wave, so that the initial conditions are $(p(x,0),h(x,0)) = (p_s,h_s) + \varepsilon \cdot \mathrm{Re}[(p_e,h_e)\exp(-\lambda x)]$, where $\varepsilon << 1$, λ is the unstable eigenvalue of (14) at (p_s,h_s), which is unique up to complex conjugacy, and (p_e,h_e) is the corresponding normalised eigenvector. The prey density in the reaction-diffusion solution evolving from this initial condition is shown at three different times (—), and compares extremely well with the oscillations observed behind the invasive wave, for the same parameters (- - -). In the latter solution, an appropriate spatial translation is applied at one time point in order to give correspondence between the two sets of solutions. A similarly good comparison is observed for the predator density and for other sets of parameter values. In the case illustrated, the kinetics are as in Fig. 3, with $D_p = D_h = 1$, $A = 3$, $B = C = 0.1$, $\varepsilon = 0.005$.

pairs of eigenvalues, with positive and negative real parts. Thus the wave oscillates in space with an exponentially decaying amplitude as it approaches the steady state; in fact these oscillations play no significant role and it is the exponential decay rate that counts. Having calculated the form of this approach, I use it as the initial condition for a numerical solution of the PDEs (13). This numerical solution does not simulate invasion, it is simply a "numerical experiment", to test the behaviour that results from these decaying initial conditions. The simulation is exactly of the type discussed in Section 2, except that there are spatial oscillations in the initial data, as well as exponential decay. As expected, these decaying initial conditions evolve to periodic travelling waves. But crucially, the particular periodic wave selected is exactly that seen in the wave of invasion, for the same parameters; the comparison is illustrated for one case in Fig. 5, and is equally good for a wide range of other parameters and kinetic terms (SHERRATT, 1994b; SHERRATT *et al.*, 1995a).

From an ecological perspective, the model predicts that spatiotemporal oscillations arise quite naturally behind invasion. However, reaction-diffusion models alone provide a rather weak base of evidence for making such a sweeping statement, in view of the important role played by spatial and temporal discretisation in many ecological systems. In fact, my collaborators and I (SHERRATT *et al.*, 1995b) have recently shown that the same phenomenon of regular oscillations behind invasion arises in a number of spatially and/or temporally discrete models, as well as in the reaction-diffusion model discussed here, suggesting that this phenomenon may well occur in real predator-prey systems.

4. A Route to Chaos

In the previous two sections, I have discussed mechanisms in which periodic travelling waves are generated naturally. In both cases, the particular periodic wave observed is selected from the continuum of possible waves by a definite, albeit slightly complex, mechanism. However, in Section 1, I mentioned the question of periodic wave stability: amongst the continuum of possible periodic waves, only some are stable as reaction-diffusion solutions. This leads to a natural question: is it possible that the wave selection rules described in Sections 2 and 3 can lead to the selection of an unstable wave? The answer to this question is a definite "yes", and in this section I will discuss the nature of the solutions that arise in such cases.

To begin my discussion of this stability issue, I return to the λ-ω systems (3). In this case, I have derived a formula (9) for the periodic wave amplitude $\hat{r}$ that evolves from exponentially decaying initial conditions; in this formula, s is related to the initial decay rate ξ by (11). This means that the stability of the resulting waves can be determined very easily, using KOPELL and HOWARD's (1973) stability condition (5). To be specific, I consider the particular case $\lambda(r) = 1 - r^p$, $\omega(r) = b(\omega_0 - r^p)$, where p is a positive parameter. Then (9) implies that

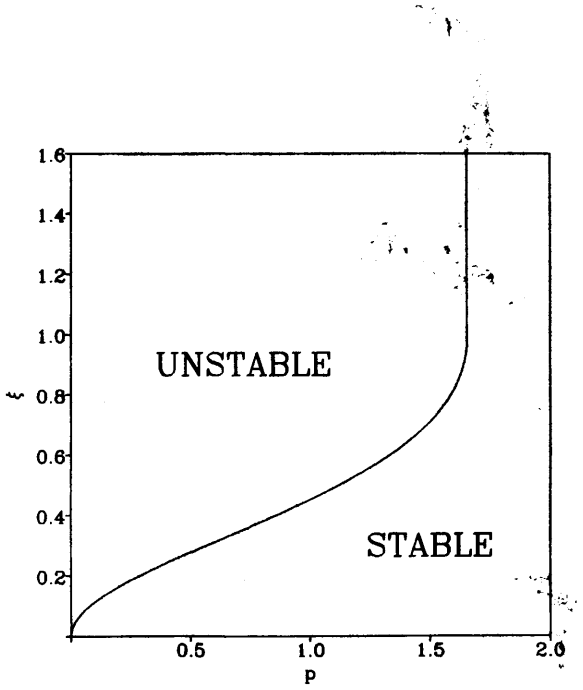

Fig. 6. An illustration of the condition (16) for the stability of periodic waves generated by initial conditions (6) for the λ-ω system (3), with $\lambda(r) = 1 - r^p$ and $\omega(r) = \omega_0 - r^p$. Thus in terms of the notation in the main text, the case illustrated is for $b = 1$.

$$\hat{r} = \left[\frac{1}{2b^2}\left(\left\{s^4 + 4b^2s^2\right\}^{1/2} - s^2\right)\right]^{1/p}, \tag{15}$$

and using (11), the stability condition (5) becomes

$$\xi > \left[p^2 + 4\left(1+b^2\right)p\right]^{-1}\left[2b\left(1+b^2\right) - \sqrt{4b^2\left(1+b^2\right)^2 - 4\left(1+b^2\right)p - p^2}\right] \tag{16a}$$

and

$$p < 2\left(1+b^2\right)\left(\sqrt{1+b^2} - 1\right) \tag{16b}$$

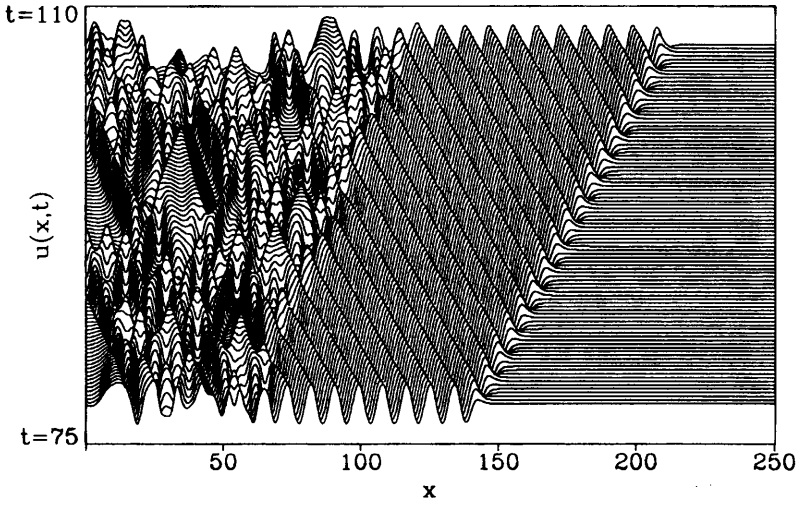

Fig. 7. A space-time plot of the numerical solution for $u(x,t)$ of (3) with $\lambda(r) = 1 - r^2$ and $\omega(r) = 3(1 - r^2)$. The equation is solved on a large domain $0 \le x \le x_\infty$, subject to $u = v = 0$ at $x = x_\infty$ and with the symmetry condition $u_x = v_x = 0$ at $x = 0$. The boundary condition at $x = 0$ essentially plays no role and simply enables the use of a semi-"infinite" rather than "infinite" domain, thus reducing the computer time required for solution. The domain length x_∞ is taken to be sufficiently large that further increase has a negligible effect on the solution over the time interval concerned. The numerical method is described in Fig. 2, and a space mesh of 1001 equally spaced points was used, with $x_\infty = 250$. At $t = 0$, u and v were set to 0.1 at the first mesh point (on the $x = 0$ boundary), with $u = v = 0$ at the other mesh points; however, the solution is essentially the same for any initial perturbation that is localised in space (i.e. "$\xi = \infty$"), as discussed in the main text. The solution is plotted as a function of x at successive times in the range $75 \le t \le 110$, with the vertical separation of solutions proportional to the time interval between them. The solution for v is qualitatively similar to that for u.

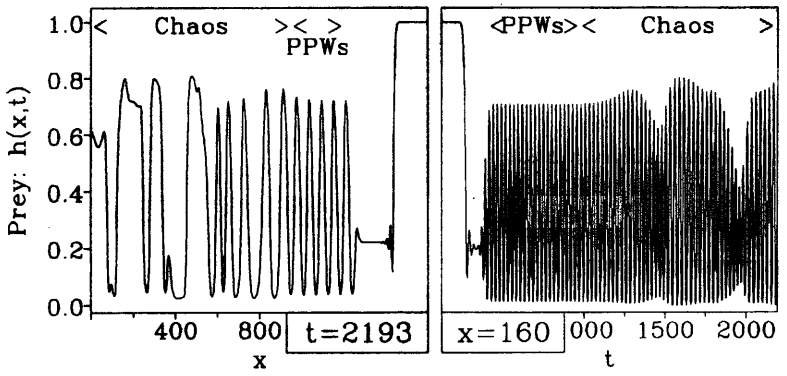

Fig. 8. The spatial and temporal variations in prey densities behind a wave of invasion by predators, for parameters on the borderline between regular and irregular oscillations. The qualitative form of the predator distributions behind the invading front are very similar. Immediately behind the invading front, there are regular spatiotemporal oscillations, corresponding to periodic plane waves (PPWs). However, these periodic plane waves are just unstable, and further back from the front, instabilities have had time to grow, giving rise to irregular behaviour. The kinetics are $f_p(p,h) = B_p(A - 1 - Ae^{-Ch})$, $f_h(p,h) = h(1 - h) - p(1 - e^{-Ch})$, which is a standard predator-prey model (MAY, 1981), and the parameters are $D_p = D_h = 1$, $A = 1.5$, $B = 0.22$, $C = 5$.

for stability. This condition is illustrated in Fig. 6.

When p and ξ are in the unstable regime, numerical solutions of the reaction-diffusion equations (3) subject (6) again consist of a wave front moving across the domain. Immediately behind the front is a band of periodic travelling waves, of amplitude given by (15); however these waves are unstable and behind the leading band of periodic waves the solution consists of irregular oscillations, arising from this instability. A typical solution is illustrated in Fig. 7.

For reaction-diffusion systems not of λ-ω form, there is no analytical analogue of the stability formula (16): to derive such an analogue would require a formula for the predicted periodic wave and a formula for periodic wave stability, both of which are lacking. However, numerical solutions have the same qualitative form as in the λ-ω case for a wide range of systems, including in particular the calcium signalling model (12) discussed in Section 2.

In the case of periodic waves behind invasion, I have again to rely on numerical observation, but the form of the solutions is qualitatively very similar. A typical case for a predator-prey model is illustrated in Fig. 8. Behind the invasive wave front there is a band of periodic waves, and further back these degenerate into irregular oscillations. In many cases, there is in fact no visible band of periodic waves, with irregular oscillations immediately behind the invasive front. I hypothesise that this is because although periodic waves do form, they destabilise so fast that they are never actually seen; however, it is very difficult to verify this using numerical tests.

The major outstanding issue concerns the nature of the irregular oscillations. Is this

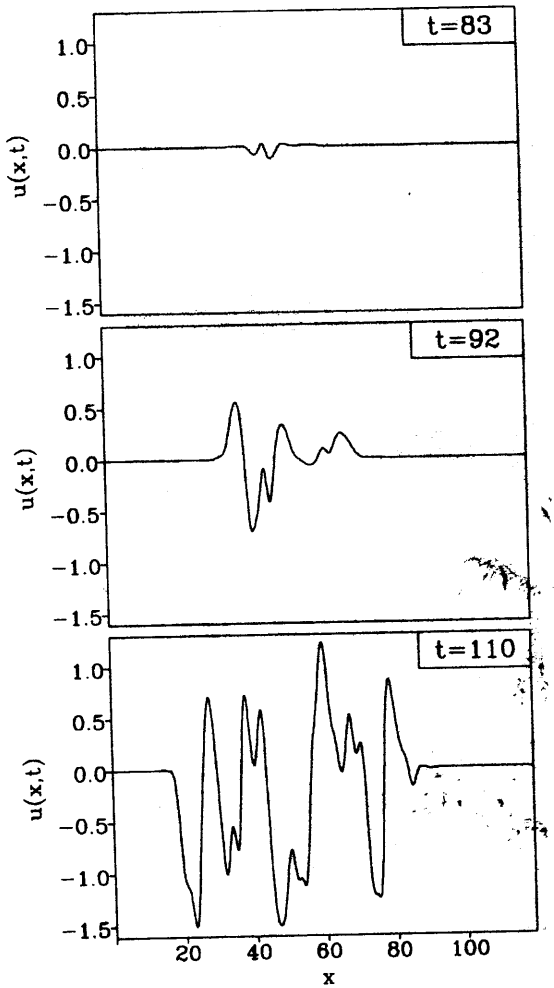

Fig. 9. The evolution of a small perturbation applied to the irregular wake region in the solution illustrated in Fig. 7. The solution was solved up to a time $t = 75$ exactly as described in the legend to Fig. 7, obtaining the solution at the first time illustrated there. I then continued the solution for two sets of initial conditions, one without any perturbation (simply the continuation of the numerical solution), and the other with a small perturbation applied to the middle of the irregular region: specifically 0.01 was added uniformly to u and v at all space points in the region $49 < x < 51$. The figure illustrates the development of this perturbation, calculated as the difference between the two solutions. The perturbation both grows and expands spatially as time increases. I plot only the difference in the u solutions; however the difference in the v solutions develops in a qualitatively similar way.

an example of spatiotemporal chaos, or is there some underlying order? I have used two essentially unrelated approaches to investigate this, both numerical. The first approach is very simple: I apply a small, spatially localised perturbation to a region of irregular oscillations, and follow its evolution in space and time. In a wide range of cases, the results

are the same; the perturbation grows and expands in both directions away from its original location (Fig. 9). This implies a sensitivity to perturbations that is characteristic of chaotic behaviour; when corresponding perturbations are applied to stable periodic waves, they decay very rapidly.

My second approach to studying the nature of the irregular oscillations is an attempt to find bifurcation sequences that are recognisable as traditional routes to chaos. To do this I have focussed on λ-ω systems, and considered numerical solutions on a relatively small finite domain. On such a domain, periodic travelling waves will only occur for slightly unusual boundary conditions, and I impose $r_x = 0$ and $\theta_x = \sqrt{\lambda(r^*)}$. Here r and θ are polar coordinates in the u-v plane, as explained in Section 2, and r^* is a positive constant. These boundary conditions mean that the periodic wave of amplitude r^* is a solution for any domain length. I then considered varying r^*, for a fixed domain length and a particular $\lambda(.)$ and $\omega(.)$, and studying the corresponding variation in the long-term numerical solution of (3). This is a very expensive numerical procedure and I have only considered one λ-ω system in detail, namely $\lambda(r) = 1 - r^2$, $\omega(r) = 3 - r^2$. The full results of this study are presented elsewhere (SHERRATT *et al.*, 1995b; SHERRATT, 1995), and I will only summarise them here. When r^* is close to one, the periodic wave of amplitude r^* is stable. However, as r^* decreases, the wave becomes unstable, and the long-term behaviour changes from constant r and θ_x to periodic temporal oscillations at all space points. As r^* is decreased further these periodic oscillations in r and θ_x themselves lose stability, and double in period. This is the onset of a period doubling cascade leading to temporally irregular oscillations. For even smaller values of r^* there is a window of regular behaviour followed by a series of bifurcations to tori, which again lead to irregular behaviour.

These observations have intrinsic interest from a dynamical systems viewpoint, but in the context of the present paper, the key result is simply the observation of a period doubling cascade and bifurcations to tori. These are well-known routes to chaos in ordinary differential equations, and provide strong evidence that the irregular oscillations observed in these finite domain computations are temporally chaotic. In the case of irregularities in the wave of evolving periodic waves, whether from exponentially decaying initial data or behind invasive wave fronts, the situation is of course slightly more complex, because the spatial domain occupied by the irregular oscillations is continually growing. Thus the spatiotemporal irregularities in these cases are in fact perpetual transients in a progression towards chaos.

5. Conclusions

Periodic travelling waves are a fundamental solution form of oscillatory reaction-diffusion equations in one space dimension. I have discussed ways in which these waves arise naturally in oscillatory systems, and have explained the rather complex mode selection procedure by which a particular wave is selected from the continuum of possible waves. I have also described the way in which the selection of an unstable wave can result in the natural generation of spatiotemporal irregularities from quite regular initial

conditions, and have presented evidence that these irregularities are in fact an example of spatiotemporal chaos. These results have two basic types of application. The first of these are mathematical applications, providing important insight into the dynamical structure of oscillatory reaction-diffusion equations, with particular implications for the study of two-dimensional solution forms such as spiral waves and target patterns. The second area of application is oscillatory biological and ecological systems. In particular, the results make specific predictions for intracellular calcium signalling and predator-prey invasion, which I have discussed. Many other biological and chemical systems are also oscillatory, and the behaviour I have discussed may also be important in a number of these other systems.

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