BOUNDS ON COMPLEXITY IN REACTION-DIFFUSION SYSTEMS

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1. Introduction.

We consider equations of the form

$$(1.1) \qquad \underset{\sim}{u}_t : F(\underset{\sim}{u},\underset{\sim}{x}) + \underset{\sim}{D}\Delta\underset{\sim}{u} \quad ,$$

$\underset{\sim}{u} \in \mathbb{R}^n$, $\underset{\sim}{x}$ in a bounded region $\Omega \subset \mathbb{R}^m$. Here $\underset{\sim}{D}$ is a positive diagonal matrix of diffusion coefficients and F is C^1 smooth in both its arguments. We consider both Dirichlet and Neumann boundary conditions.

Under very general assumptions, we shall give rigorous upper bounds on the complexity of solutions to (1.1), both in space and in time, with estimates that are proportional to the volume of Ω . Our notions of complexity, which will be detailed below, involve rates of growth of small perturbations of solutions to (1.1). It will be seen that the diffusion term $\underset{\sim}{D}\Delta\underset{\sim}{u}$ in (1.1) limits complexity, just as the term $-h^2\Delta/2m$ does in the Schrödinger equations; indeed, quantum mechanical estimates will be used to bound the relevant growth rates.

The estimates to be derived are valid for any set of equations (1.1) satisfying a mild compactness condition :

(1.2) Equation (1) admits a positively invariant region [27], i.e., there exists a compact set $K \subset \mathbb{R}^n$ such that, for any solution $u(x,t)$ having all its boundary and initial values in K , $u(x,t) \in K$ for all t for which $u(x,t)$ is defined.

In connection with a local existence theorem [27], condition (1.2) provides a-priori estimates which ensure global existence and uniqueness. This condition holds for many important systems of reaction-diffusion equations; for examples and methods of constructing such a K , see [27]. We shall assume initial conditions in the space $L^2(\Omega, \mathbb{R}^n)$.

We shall be most interested in equations (1.1) for which some solutions are known to have complicated spatial and temporal behavior. These include systems for which the reaction equation

$$(1.3) \qquad \underset{\sim}{u}_t = F(\underset{\sim}{u},\underset{\sim}{x})$$

has a limit cycle for some set of $\underset{\sim}{x} \in \Omega$. We have in mind, for example, equations (1.3) which model the kinetics of the Belousov-Zhahotinskii reagent, an oscillating chemical reaction. (Both the realistic Field-Noyes model [10] and the simple "λ-ω" caricature [16], [14], [15], [12], [13], [3] satisfy condition (1.2) under appropriate assumptions on $\underset{\sim}{D}$ [27]). It is well accepted that only reaction and diffusion are involved in the formation of the complicated patterns which develop when this fluid is allowed to sit in a thin layer (and covered to prevent convection). These patterns may include spirals and/or "target patterns" (described in Section 5), as well as thin transition or "shock" regions between these subpatterns (targets or spirals). As discussed in Section 5, the bounds provide upper limits to the number of coherent subpatterns per unit of area. One feature of these bounds is that they can be independent of the scale of spatial variation in the kinetics (1.3). Thus, though the formation of the target patterns is known to be facilitated by the addition of impurities [29], there may be an upper bound to the density of these subpatterns independent of the distribution of the impurities. Other applications are also discussed in Section 5.

Similar estimates were made in Ruelle [25], Babin and Vishik [1], Constantin and Foias [4], Ruelle [26] for (the more difficult case of) the Navier-Stokes equations, and used to get upper bounds for the entropy and the Hausdorff dimension of the attracting set. The latter numbers are measures, respectively, of the temporal and spatial complexity of the time-averaged solutions. The notions to be used in this paper, which will be described in Section 2, are more general in the sense that they measure instantaneous rather than asymptotic complexity. However, as shown in the Appendix, the time-averaged versions of these concepts are bounds for the entropy and the Hausdorff dimension, and similar methods give bounds on these as well.

The reason for using non-asymptotic notions is that patterns in reaction-diffusion systems are constantly changing and, over a very long time scale may simplify. (For example, in the Belousov-Zhabotinskii (BZ) reagent, the number of target patterns decreases over time as some of them are taken over by, and merged into, other target patterns). Thus, we seek a theory that can quantify complexity of the "metastable" solutions, rather than the final attracting sets.

The paper is organized as follows : In Section 2, we discuss our notions of spatial and temporal complexity. The main results are given in Section 3. For Dirichlet conditions, we use quantum-mechanical estimates to compute these bounds. For rectangular domains with either Dirichlet or Neumann conditions, other estimates are provided in Section 4. In Section 5 bounds are explicitly calculated for a simple example. Section 6 contains a discussion of applications, and the connection of this paper to previous results of Conway et. al [5] on the non-existence of spatial structure in small domains. The appendix extends the results to infinite time, and gives the connection between Section 2 and ergodic theory.

2. Measures of spatial and temporal complexity.

Small perturbations $\underset{\sim}{\varphi}$ of $\underset{\sim}{u}$ satisfy the linearized equation

$$(2.1) \qquad \underset{\sim}{\varphi}_t = \underset{\sim}{D}\Delta\underset{\sim}{\varphi} + dF\cdot\underset{\sim}{\varphi}$$

where dF is the $n \times n$ matrix $\partial F/\partial\underset{\sim}{u}$. Note that Dirichlet boundary conditions on $\underset{\sim}{u}$ imply that $\underset{\sim}{\varphi}|\partial\Omega = 0$. Neumann conditions for n imply homogeneous Neumann conditions for $\underset{\sim}{\varphi}$. We introduce the L^2 norm

$$\|\underset{\sim}{\varphi}\| = [\int(\sum_{i=1}^{n} \varphi_i^2)dx]^{1/2}$$

where $\underset{\sim}{\varphi} = (\varphi_1,\ldots,\varphi_m)$. The instantaneous rate of growth of $\|\varphi\|$ is

$$\frac{d}{dt}\log\|\underset{\sim}{\varphi}\| = \frac{1}{\|\underset{\sim}{\varphi}\|}\frac{d}{dt}\|\varphi\| = \frac{1}{\|\varphi\|^2}(\underset{\sim}{\varphi}, \underset{\sim}{D}\Delta\underset{\sim}{\varphi} + dF\cdot\underset{\sim}{\varphi}) \quad (2.2)$$

Here $(\cdot,\cdot)$ denotes the inner product associated with the L^2 norm. Similarly, the instantaneous rate of growth of a k-volume element is

$$\frac{d}{dt}\log\|\varphi_1 \wedge \varphi_2\wedge\cdots\wedge\varphi_k\| \quad (2.3)$$

where the exterior product $(\wedge)$ of vectors in L^2 , and their norms, are defined in the usual manner.

We take as our measure of temporal complexity the quantities

$$h_D(\underset{\sim}{u},t) =: \max_k c_D(k,\underset{\sim}{u},t)$$

or

$$h_N(\underset{\sim}{u},t) =: \max_k c_N(k,\underset{\sim}{u},t)$$

where the subscripts D and N stand, respectively for Dirichlet and Neumann, and

$$c(k,\underset{\sim}{u},t) =: \max_{\underset{\sim}{\varphi}_1\wedge\cdots\wedge\underset{\sim}{\varphi}_k} \frac{d}{dt}\log \underset{\sim}{\varphi}_1\wedge\cdots\wedge\underset{\sim}{\varphi}_k \quad (2.4)$$

with $c(k,\underset{\sim}{u},t)$ equal to c_D or c_N . Similarly we shall use $h(\underset{\sim}{u},t)$ to denote either h_D or h_N . $h(\underset{\sim}{u},t)$ may be viewed as the sum of the rates of growth of the unstable modes of the system. It is also the "instantaneous" concept whose asymptotic analogue is a bound for topological entropy [25], [26]. This will be discussed in the Appendix. We note for now that the growth of small perturbations to solutions of (1.1) corresponds to sensitive dependence on initial conditions, and $h(\underset{\sim}{u},t)$ indicates how much of this is present at time t .

(However, the existence of this sensitive dependence at some finite time does not indicate what is normally called "chaos" since the rate of growth of perturbations may decay as $t \to \infty$).

We shall take as the measure of spatial complexity $d(\underset{\sim}{u},t)$ a quantity which is an upper bound for the number of unstable and neutrally stable modes, and whose asymptotic analogue can be interpreted as a bound for Hausdorff dimension of the attracting set in $L^2(\Omega, \mathbb{R}^n)$ of (1.1). Let $c(s,\underset{\sim}{u},t)$, $s \geq 0$ be defined from (2.4) by linear interpolation between successive integer values of s . Then

$$d_D(\underset{\sim}{u},t) =: \max\{s : c_D(s,\underset{\sim}{u},t) \geq 0\} \quad ,$$

(2.5)

$$d_N(\underset{\sim}{u},t) =: \max\{s : c_N(s,\underset{\sim}{u},t) \geq 0\} \quad .$$

As before, we use $d(\underset{\sim}{u},t)$ to denote either d_D or d_N .

3. Estimates of complexity.

We first show that the quantity $c_D(k,u,t)$ defined in the previous section may be estimated in terms of the eigenvalues of an associated diffusion operator $\underset{\sim}{D}\Delta+w$, where $w : \Omega \to \mathbb{R}^1$. We will then make use of estimates on these eigenvalues which come from the study of the classical limit of quantum mechanics, with $\underset{\sim}{D}\Delta+w$ interpreted as a Schrödinger operator (up to sign).

The associated "potential" w is not unique. We first let the matrix $\underset{\sim}{W}$ be the symmetric part of dF , i.e. , $\underset{\sim}{W} = \frac{1}{2}(dF+(dF)^*)$, where $*$ denotes adjoint. (Here $\underset{\sim}{W}$ depends on $\underset{\sim}{x}$ and t through its dependence on a solution $\underset{\sim}{u}$ of (1.1); since we are concerned with instantaneous rate of growth at fixed t , we ignore the dependence on t). Let $w = w(x)$ be an upper bound for $\underset{\sim}{W}$, i.e. any scalar such that the matrix $w\underset{\sim}{I}-\underset{\sim}{W}$ is a non-negative operator. ($\underset{\sim}{I}$ is the $n \times n$ identity matrix. (The best choice is $w(x) = \lambda(x)$, where λ is the largest eigenvalue of $\underset{\sim}{W}$; one may also take the uniform norm $|dF(x)|$ of the matrix dF , or $[\sum_{i,j} W_{ij}^2]^{1/2}$, where W_{ij} is the i,j^{th} component of $\underset{\sim}{W}$). For any such w , (2.2) implies

$$(3.1) \qquad \frac{d}{dt} \log \|\underset{\sim}{\varphi}\| = \frac{1}{\|\underset{\sim}{\varphi}\|^2} (\underset{\sim}{\varphi}, \underset{\sim}{D}\Delta\underset{\sim}{\varphi}+W\underset{\sim}{\varphi}) \leq \frac{1}{\|\underset{\sim}{\varphi}\|^2} (\underset{\sim}{\varphi}, \underset{\sim}{D}\Delta\underset{\sim}{\varphi}+w\varphi) \quad .$$

Remark: For the estimates that will follow, it is desirable to have w as small as possible. The upper bound $w(x)$ is not independent of changes of coordinates, and hence could possibly be improved by a linear change $\underset{\sim}{\varphi} \to \underset{\sim}{A}\,\underset{\sim}{\varphi}$. However, we require that $\underset{\sim}{D}$ be preserved under this change, and hence that $\underset{\sim}{A}$ commute with $\underset{\sim}{D}$. For simple systems, it may be possible by inspection to get a better bound (see Section 5).

Now consider $\underset{\sim}{D}\Delta+w$ as an operator on $L^2(\Omega, \mathbb{R}^n)$ with $\underset{\sim}{\varphi}|\partial\Omega = 0$; let a_1 be the largest eigenvalue. From (3.1) it follows that

$$(3.2) \qquad \frac{d}{dt} \|\log \underset{\sim}{\varphi}\| \leq a_1 \quad .$$

Similarly, the instantaneous rate of growth of a k-dimensional volume element $\|\varphi_1 \wedge \varphi_2 \wedge \cdots \wedge \varphi_k\|$ under the evolution of (1.1) is also bounded in terms of the eigenvalues of $\underset{\sim}{D}\Delta+w$:

Lemma 1 : Let $a_1 \geq a_2 \geq \cdots \geq a_k \geq \cdots$ be the eigenvalues of $\underset{\sim}{D}\Delta+w$ in decreasing order, then

$$\frac{d}{dt} \log \|\varphi_1 \wedge \cdots \wedge \underset{\sim}{\varphi}_k\| \leq a_1+a_2+\cdots+a_k \ .$$

The exterior products $(\wedge)$ of vectors in a Hilbert space, and their norms, are defined in the standard way, and Lemma 1 is proved in the same manner as (3.2). (See [25]).

The rest of the estimates for c_D and d_D make use of semi-classical formulae for the eigenvalues of scalar operators :

Proposition 1 : Let $D > 0$ be a scalar and $w : \Omega \to \mathbb{R}$. Let $b_1 \geq b_2 \geq \ldots$ be the eigenvalues of $D\Delta + w$, acting on $L^2(\Omega, \mathbb{R})$, where $\Omega \subset \mathbb{R}^m$ is bounded, and zero boundary conditions are imposed on $\partial\Omega$. Then

a) The sum of the positive eigenvalues $b_i \geq 0$ satisfies

(3.4) $$\sum_{b_i > o} b_i \leq L_m D^{-m/2} \int_\Omega w^{1+m/2} dx \ .$$

Here L_m is a universal constant depending only on the dimension m of the spatial domain. The best estimates of L_m currently known are

$$L_1 \leq \frac{4}{3} \ , \quad L_2 \leq .24008 \ , \quad L_3 \leq .040304$$

b) Let $c^*(k) = \sum_{i=1}^{k} b_j$, and let $c^*(s)$ be defined for all $s \geq 0$ by linear interpolation between integers. Let

(3.5) $$d^* = \max\{ s \ : \ c^*(s) \geq 0\} \quad .$$

Then

(3.6) $$d^* \leq A_m D^{-m/2} |\Omega|^{2/(m+2)} [\int_\Omega w^{1+m/2}]^{m/(m+2)}$$

As before, the A_m are universal constants, and are estimated by

$$A_1 \leq 2.050 \qquad A_2 \leq .5597 \qquad A_3 \leq .1329$$

Proof : Part a) is in Lieb and Thirring [20]. Part b), in conjectural form in [25], is proved in [19]. Lieb's proof uses an estimate of the form

(3.7) $$c^*(s) \leq c_1(D,s) \equiv D^{-\frac{m}{2}} c_2(D^{\frac{m}{2}} s)$$

with concave c_2 (this fact will be used below). One shows that

$$\max\{s : c_2(s) \geq 0\} \leq |\Omega|^{\frac{2}{m+2}} [\int_\Omega w^{1+\frac{m}{2}}]^{\frac{m}{m+2}} .$$

We now relate the quantities estimated in Proposition 1 to $h_D(u,t)$ and $d_D(u,t)$. Let $0 < D_1 \leq D_2 \leq \cdots \leq D_n$ be the eigenvalues of the diagonal matrix $\underset{\sim}{D}$, $w : \Omega \to R^1$ an upper bound (for each $\underset{\sim}{x} \in \Omega$) on $\underset{\sim}{W} = \frac{1}{2}(dF+(dF)^*)$, and $b_1^i \geq b_2^i \geq \ldots$ be the eigenvalues of the operator $D_i\Delta+w$ acting on $L^2(\Omega, \mathbb{R})$ with zero boundary conditions.

The estimates on $h_D(u,t)$ and $d_D(u,t)$ are then given by

Theorem 1. Under the conditions (1.2) of the introduction we have

$$(3.8) \qquad a) \quad h_D(u,t) \leq \sum_{i=1}^{n} \sum_{j:b^i_j \geq o} b^i_j \leq L_m(\sum_i D_i^{-m/2}) \int_\Omega w^{1+m/2} dx$$

$$(3.9) \qquad b) \quad d_D(u,t) \leq A_m(\sum_i D_i^{-m/2}) |\Omega|^{\frac{2}{m+2}} [\int_\Omega w^{1+\frac{m}{2}} dx]^{\frac{m}{m+2}}$$

Proof. Part a) follows from Lemma 1 and part a) of Prop. 1. To prove part b) we use (3.7) :

$$\begin{aligned} d_D(u,t) &\leq \max\{s_1+\cdots+s_n : c_1(D_1,s_1)+\cdots+c_1(D_n,s_n) \geq 0\} \\ &= \max\{\Sigma s_i : \Sigma D_i^{-\frac{m}{2}} c_2(D_i^{\frac{m}{2}} s_i) \geq 0\} \\ &= \sum_i D_i^{-\frac{m}{2}} \max\{s : c_2(s) \geq 0\} \\ &\leq A_m(\sum_i D_i)^{-m/2} |\Omega|^{\frac{2}{m+2}} [\int_\Omega w^{1+\frac{m}{2}} dx]^{\frac{m}{m+2}} \end{aligned}$$

as in the proof of part b) of Prop. 1.

Corollary. Define

$$M = \max_{x\in\Omega} \max_{u\in K} w(u,x) \tag{3.10}$$

(for one of the choices of w this is $M = \max_{x,u} |dF|$) . We have then

$$c(1,u,t) = \max_{\underset{\sim}{\varphi}} \frac{d}{dt} \log \|\underset{\sim}{\varphi}\| \leq M$$

$$h_D(u,t) \leq L_m (\sum_i D_i^{-m/2}) |\Omega| M^{1+m/2}$$

$$d_D(u,t) \leq A_m (\sum_i D_i^{-m/2}) |\Omega| M^{m/2}$$

If $m = 1$, we may replace L_1 , A_1 in these formulae by $2/3\pi$ and $\sqrt{3}/\pi$ respectively. This is because in one dimension, Ω is always "cubic"; see next section.

4. The special case of cubic boxes, Dirichlet and Neumann boundary conditions.

If Ω is rectangular, we may estimate directly the eigenvalues of $D\Delta+M$, both for Dirichlet and Neumann boundary conditions, without resorting to Proposition 1. The results obtained have sharper constants than the above corollary, but are less powerful than the theorem, because they use M rather than $\int w^{1+m/2}$. For simplicity we assume that Ω is a cube of side L .

The eigenfunctions of $D\Delta+M$ in the cube $\Omega = \prod_1^m [0,L]$ are of the form $\prod_1^m \sin \frac{\pi\xi_i x_i}{L}$ with integers $\xi_i > 0$ in the case of Dirichlet boundary conditions, and $\prod_1^m \cos \frac{\pi\xi_i x_i}{L}$ with integer $\xi_i \geq 0$ in the case of Neumann boundary conditions.

The sum of the largest k eigenvalues of $D\Delta+M$ satisfies therefore

$$c_D^*(k) \quad \text{or} \quad c_N^*(k) = \sum_\xi (M - \frac{D\pi^2}{L^2} |\xi|^2)$$

where the sum extends over k allowed points $\xi = (\xi_1,\ldots,\xi_m)$ closest to the origin.

We get an upper bound for $c_D^*(k)$ by spreading the unit mass located at $(\xi_1,\ldots,\xi_m)$ uniformly on the unit cube $\prod_1^m [\xi_i-1,\xi_i]$ a still higher upper bound is obtained by replacing the union of cubes by a piece of sphere (ball) of the same volume :

$$c_D^*(k) \leq \int (M - \frac{D\pi^2}{L^2} |\xi|^2) d\xi$$

The integration is over the part $\xi_1 \geq 0,\ldots,\xi_m \geq 0$ of the ball centered at the origin, with radius R such that $2^{-m}\sigma_m R^m = k$ (where σ_m is the volume of the m-ball of unit radius). If $c_D^*(s)$ is defined for real $s \geq 0$ by linear interpolation between integers, the same argument applies, k being simply replaced by s in the formula.

To evaluate $c_N^*(k)$ we spread the unit mass located at $(\xi_1,\ldots,\xi_m)$ uniformly on the unit cube $\prod_1^m [\xi_i,\xi_i+1]$, obtaining

$$c_N^*(k) \leq \int (M - \frac{D\pi^2}{L^2} [\max(|\xi|-\sqrt{m},0)]^2) d\xi$$

where the integral is over the same region as above. Again we may replace k by a real number $s \geq 0$.

The angular integrations in the above estimates are trivial, so that one may replace $d\xi$ by $\frac{\sigma_m}{2^m} d|\xi|^m$. Writing $\lambda = (\frac{D}{M})^{1/2} \frac{\pi}{L} |\xi|$ we obtain

(4.1) $$c_D^*(s) \leq \frac{\sigma_m}{2^m} \cdot m(\frac{ML^2}{D\pi^2})^{\frac{m}{2}} \cdot M \int_0^\tau ((1-\lambda^2)\lambda^{m-1} d\lambda$$

(4.2) $$c_N^*(s) \leq \frac{\sigma_m}{2^m} . m(\frac{ML^2}{D\pi^2})^{\frac{m}{2}} . M$$

$$[\int_0^{\tau_o} \lambda^{m-1} d\lambda + \int_{\tau_o}^{\tau} (1-(\lambda-\tau_o)^2)\lambda^{m-1} d\lambda]$$

where

$$(4.3) \qquad \tau_o = \left(\frac{Dm\pi^2}{ML^2}\right)^{1/2}$$

and $\tau = \left(\frac{D\pi^2}{ML^2}\right)^{1/2} \left(\frac{2^m s}{\sigma_m}\right)^{1/m}$. The largest τ for which (4.1) and (4.2) are non negative are respectively given by

$$\frac{\tau^{m+2}}{m+2} - \frac{\tau^m}{m} = 0$$

and

$$\frac{\tau^{m+2}}{m+2} - \frac{\tau^m}{m} = \frac{2\tau_o \tau^{m+1}}{m+1} + \text{higher order in } \tau_o$$

We have thus

$$\max\{s : c_D^*(s) \geq 0\} \leq \left(1+\frac{2}{m}\right)^{m/2} \left(\frac{ML^2}{D\pi^2}\right)^{m/2} \frac{\sigma_m}{2^m}$$

$$\max\{s : c_N^*(s) \geq 0\} \leq \left[\left(1+\frac{2}{m}\right)^{m/2} + O(\tau_o)\right] \left(\frac{ML^2}{D\pi^2}\right)^{m/2} \frac{\sigma_m}{2^m}$$

and changing from Dirichlet to Neumann boundary condition is a small correction when τ_o is small. In the Dirichlet case we may write

$$D_D^* = \max\{s : c_D^*(s) \geq 0\} \leq A_m^c \, D^{-m/2} |\Omega| M^{m/2}$$

where

$$(4.4) \qquad A_m^c = \left(1+\frac{2}{m}\right)^{\frac{m}{2}} \frac{\sigma_m}{2^m} \pi^{-m} = \begin{cases} \frac{\sqrt{3}}{\pi} & \text{for } m = 1 \\ \frac{1}{2\pi} & \text{for } m = 2 \\ \left(\frac{5}{3}\right)^{3/2} \frac{1}{6\pi^2} & \text{for } m = 3 \end{cases}$$

To estimate the sum of the positive eigenvalues of $D\Delta + M$ we take $\tau = 1$ in (4.1) or $\tau = 1+\tau_o$ in (4.2), and find that the sum is

$$(4.5) \qquad \leq L_m^c \, D^{-m/2} |\Omega| M^{1+m/2}$$

in the Dirichlet case, with

$$(4.6) \qquad L_m^c = \frac{2}{m+2} \cdot \frac{\sigma_m}{2^m} \pi^{-m} = \begin{cases} \frac{2}{3\pi} \\ \frac{1}{8\pi} \\ \frac{1}{15\pi^2} \end{cases}$$

In the Neumann case there are again $O(t_o)$ corrections to (4.5)

<u>Theorem 2</u>. Under the conditions (1.2) of the introduction, if Ω is cubic one may write

$$(4.7) \qquad h_D(u,t) \leq L_m^c(\sum_i D_i^{-m/2})|\Omega|M^{1+m/2}$$

$$(4.8) \qquad d_D(u,t) \leq A_m^c(\sum_i D_i^{-m/2})|\Omega|M^{m/2}$$

with the definitions (3.10), (4.4), (4.6) and

$$(4.9) \qquad h_N(u,t) \leq L_m^N(\sum_i D_i^{-m/2})|\Omega|M^{1+m/2}$$

$$(4.10) \qquad d_N(u,t) \leq A_m^N(\sum_i D_i^{-m/2})|\Omega|M^{m/2}$$

where L_m^M, A_m^N now depend on Ω, but differ from L_m^c, A_m^c only by terms of order $O(\tau_o)$ with τ_o given by (4.3).

5. <u>A simple example</u>.

We consider the reaction-diffusion equation

$$(5.1) \qquad \underset{\sim}{u}_t = \begin{pmatrix} \lambda & -\omega \\ \omega & \lambda \end{pmatrix} \underset{\sim}{u} + D\Delta\underset{\sim}{u} \qquad \underset{\sim}{u} \in \mathbb{R}^2 , \quad D \in \mathbb{R}^1$$

where $\lambda = k(1 - \frac{|u|^2}{R^2})$, $\omega = c-k_1 \frac{|u|^2}{R^2} + g(x)$, and $g : \Omega \to \mathbb{R}$ is a smooth function. The system is enclosed in a bounded region $\Omega \subset \mathbb{R}^n$, and $\underset{\sim}{u}$ is imposed on $\partial\Omega$. The region K may be here taken to be $K = \{\underset{\sim}{u} : |\underset{\sim}{u}| \leq R\}$.

The symmetrized matrix $\underset{\sim}{W}$ of the linearization of (5.1) has components

$$W_{11} = k(1 - \frac{|u|^2}{R^2}) - \frac{2k}{R^2} u_1^2 + \frac{2k_1}{R^2} u_1 u_2$$

$$W_{22} = k(1-\frac{|u|^2}{R^2}) - \frac{2k}{R^2} u_2^2 - \frac{2k_1}{R^2} u_1 u_2$$

$$W_{12} = W_{21} = \frac{-2k}{R^2} u_1 u_2 + \frac{k_1}{R^2} (u_2^2 - u_1^2)$$

It can easily be checked that for any u_1, u_2 the 2×2 matrix with i,j^{th} component $u_i u_j$ is a non-negative matrix. Hence $\underset{\sim}{W}$ is bounded above by $\underset{\sim}{\overline{W}}$ with components

$$\overline{W}_{11} = k(1 - \frac{|u|^2}{R^2}) + \frac{2k_1}{R^2} u_1 u_2$$

$$\overline{W}_{22} = k(1 - \frac{|u|^2}{R^2}) - \frac{2k_1}{R^2} u_1 u_2$$

$$\overline{W}_{12} = \overline{W}_{21} = \frac{k_1}{R^2} (u_2^2 - u_1^2)$$

A scalar upper bound for $\underset{\sim}{\overline{W}}$ is the largest eigenvalue of $\underset{\sim}{\overline{W}}$ or

(5.2) $$w = k(1 - \frac{|u|^2}{R^2}) + k_1 \frac{|u|^2}{R^2} \leq M = \max \{k, k_1\}.$$

Thus we have

(5.3) $$h_D(\underset{\sim}{u}, t) \leq 2L_m D^{-m/2} M^{(1+m/2)} |\Omega|$$

(5.4) $$d_D(\underset{\sim}{u}, t) \leq 2A_m D^{-m/2} M^{m/2} |\Omega|$$

In the case of cubic domains we may replace L_m, A_m by the smaller constants L_m^c, A_m^c. In particular this can always be done in the one-dimensional case $(m = 1)$. In the case of cubic domains, the Neumann boundary conditions may also be treated, using $L_m^N = L_m^c + 0\left(\frac{1}{L}\left(\frac{D}{M}\right)^{1/2}\right)$, $A_m^N = A_m^c + 0\left(\frac{1}{L}\left(\frac{D}{M}\right)^{1/2}\right)$.

Note that the bounds on h and d (which are independent of the solutions $\underset{\sim}{u}$) are in terms of the volume of Ω, the size of D and an inverse time $M = \max\{k, k_1\}$; the larger this inverse time, the more possible structure in the solution. The spatial variation in the kinetics is not reflected in the estimates. Also note that the frequencies associated with the oscillations play no role in the estimates, only the "Floquet time" given by k and the measure k_1 of frequency variation with amplitude. Furthermore, the coefficient of k in (5.2) will be small whenever the solution u is close to the limit cycle $|u| = R$. Thus, the more important time scale is given by k_1.

6. Discussion.

The existence of the upper bounds on complexity reflects the intuitively clear idea that diffusion gives lower bounds to the size of stable spatial structures. Indeed, $[d(\underset{\sim}{u},t)/|\Omega|]^{1/m}$ gives a (minimum) characteristic length scale for the size of a coherent spatial structure. However, the estimates are by no means sharp.

The estimates on the $d_N(\underset{\sim}{u},t)$ can be connected to some observed quantities (at least modulo some reasonable assumptions). For example, consider patterns in the Belousov-Zhabotinskii reagent [32]. In this oscillating reagent, phases can be identified by changes in color. If the reagent is thoroughly stirred and poured into a thin layer (and covered to prevent convection), bright blue spots form in the red medium and propagate outward. The centers of these blue spots then turn red and this also propagates outward. The process repeats with a period of the order of 2 to 3 per minute, and after a short time the entire sheet is covered with patterns of outwardly moving concentric circles known as "target patterns" (See [16] for a picture). If the liquid is sheared slightly during this process and then left alone, there emerge spiral patterns in addition to, or instead of, target patterns. A non-oscillating variant on this recipe, created by Winfree to mimic the mathematical behavior of Cardiac tissue [28], produces similar patterns. With care, one can observe the rather complex three-dimensional structure of these patterns, some topological features of which have been analyzed by Winfree and Strogatz [31].

During the formation of the target patterns/spirals (to be called sub-patterns), it seems clear that each subpattern develops independently of the others. If we make the reasonable assumption that each developing pattern corresponds to at least one unstable or neutral mode of (1.1) (with the appropriate kinetics), linearized around the solution at that time, then $d_N(\underset{\sim}{u},t)$ gives an upper bound to the number of subpatterns for a class of functions $F(\underset{\sim}{u},\underset{\sim}{x})$ for which the eigenvalues of $(dF+(dF)^*)/2$ are uniformly (over the class) bounded above independent of $\underset{\sim}{x}$, the estimates of Section 3 can be thought of as giving bounds independent of the density of impurities (as in the simple example of Section 5).

In general, structure can exist in oscillating and diffusing chemical reactions with or without the intervention of impurities. (For some of the references to this literature, see [30], [15]). Even without diffusion, however, spatial differences in frequency do lead to structure. Consider, for example, an oscillating chemical reaction carried out in a tube, with a gradient along the tube in the frequency of the underlying oscillation. (For the Belousov-Zhabotinskii reaction, this is easily accomplished by temperature gradients in a surrounding bath or chemical gradients that do not diffuse away over the time scale in question [17]). If there were no diffusion, it can be seen [17] that, starting from an initially homogeneous state, the system would evolve so as to develop waves whose wavelength becomes smaller and smaller (without limit) as t increases.

In the presence of diffusion, the wave-lengths do not become infinitely small. The estimates of Section 3 do not explicitly describe the minimal wave-length at which the decrease ends. The theory of this paper does, however, show that there are bounds on the complexity of the solution independent of the steepness of the frequency gradient. This is especially interesting because, for quite steep frequency gradients, numerical calculations (with Neumann conditions) [8] suggest that solutions do not approach any stable periodic configuration, with a fixed (common) frequency. Instead, one can get "plateaus" of frequency, i.e. intervals along the tube on which the frequency is constant, with abrupt changes of frequency in between, and the dynamics can be quite complicated. (A demonstration of this was carried out by Winfree [30], chapt. 14) on chromato-graphy paper soaked in Belousov-Zhabotinskii reagent in the presence of a tempe-rature gradient; one can explicitly see the plateaus). For an analysis of a related but spatially discrete equation, see [9].

The results of this paper may be viewed as extensions of the results of Conway et. al. on the non-existence of spatial structure for reaction-diffu-sion equations, with homogeneous Neumann boundary conditions, on domains that are sufficiently small [5]. More precisely, let $\Lambda > 0$ be the principal eigen-value of $-\Delta$ on Ω (with Neumann conditions), D_1 the smallest (positive) eigenvalue of the (positive definite) matrix $\underset{\sim}{D}$, and $M = \max\{|dF| : u \in K\}$, where $|dF|$ denotes the uniform norm of the matrix dF. Note that the compact-ness of K implies that $M < \infty$. Let $\sigma = \Lambda D_1 - M$. The following theorem says that if $\sigma > 0$, the solutions to (1.1) decay to spatially homogeneous solutions.

Theorem [5] : Consider the problem (1.1), with $F = F(u)$, $u(x,0) = u_o(x)$, and homogeneous Neumann data on $\partial\Omega$. Assume (1.1) admits a bounded invariant region K, and $\{u_o(x) : x \in \Omega\} \subset K$. If $\sigma > 0$, there are constants $c_1, c_2, c_3 > 0$ such that, for $t > 0$,

1) $\|\nabla_x u(\cdot,t)\|_{L^2} \leq c_1 e^{-\sigma t}$

2) $\|u(\cdot,t) - \overline{u}(t)\|_{L^2} \leq c_2 e^{-\sigma t}$

where

$$\overline{u}(t) = \frac{1}{|\Omega|} \int_\Omega u(x,t)dx \quad \text{and } \overline{u} \text{ satisfies}$$

$$\frac{d\overline{u}}{dt} = F(\overline{u}) + g(t) \quad , \quad \overline{u}(0) = \frac{1}{|\Omega|} \int_\Omega u_o(x)dx$$

and $g(t) \leq c_3 e^{-\sigma t}$.

Λ is inversely proportional to the squared diameter of Ω. Hence, the hypothesis $\sigma > 0$ says that diffusion (on a domain of size $|\Omega|$) is fast relative to the reaction term. The estimate (4.10) of spatial complexity is in terms of the same quantities Λ, D_1 and M (or, equivalently, $|\Lambda|$, D_1 and M).

In the Appendix we shall discuss the asymptotic versions of Sections 2 and 3, and the relation to Hausdorff dimension and entropy. For here, we note that our hypotheses imply that there is an attractor for (1.1) (with Dirichlet or Neumann conditions) in $L^2(\Omega, \mathbb{R}^n)$, and it has finite Hausdorff dimension $\dim_H$. As will be seen in the Appendix, if $w \equiv M$, then (4.8), (4.10) give bounds for $\dim_H$. Now if (1.1) is to have an attractor that is not a point $\dim_H$ must be at least 1. Thus, from (4.8), (4.10) we get

$$1 \leq A_m (\Sigma D_i^{-m/2}) |\Omega| M^{m/2}$$

where A_m denotes A_m^c or A_m^N. In conclusion,

$$(6.1) \qquad \frac{(\Sigma D_i^{-m/2})^{-\frac{2}{m}}}{|\Omega|^{2/m}} - A_m^{2/m} M \leq 0$$

which has the same form as the main hypothesis of Smoller's theorem (with the opposite sign). Thus we recover (but less sharply) Smoller's result that a necessary condition for (asymptotic) complexity is that a quantity (5.1) analogous to σ must be negative.

Appendix.

Time Averages : connecting with ergodic theory.

We now extend the theory of Sections 2,3 and 4 to allow $t \to \infty$. For $\underset{\sim}{u} : \Omega \to \mathbb{R}^n$, φ a solution to (2.1) as before, the characteristic exponent $\lambda(\underset{\sim}{u},\underset{\sim}{\varphi})$ is the following limit (if it exists) :

$$\text{(A1)} \qquad \lambda(\underset{\sim}{u},\underset{\sim}{\varphi}) = \lim_{t\to\infty} \frac{1}{t} \log \|\varphi(t)\| \quad .$$

Let f^t denote the one-parameter flow on $L^2(\Omega, \mathbb{R}^n)$ associated with (1.1), which takes the initial condition $\underset{\sim}{u}(\cdot,0)$ into $\underset{\sim}{u}(\cdot,t)$ and let $df^t_{\underset{\sim}{u}}$ be its derivative at $\underset{\sim}{u}$. The possible characteristic exponents depend on $\underset{\sim}{u} = \underset{\sim}{u}(\cdot,0)$ and are the logarithms of the eigenvalues of

$$\text{(A2)} \qquad \Lambda_{\underset{\sim}{u}} = \lim_{t\to\infty}[(df^t_{\underset{\sim}{u}})^* df^t_{\underset{\sim}{u}}]^{1/2t}$$

The limit exists. (Here * denotes the operator adjoint). Note that, if $\|\varphi\|$ grows exponentially in time, the RHS of (A1) is just the limit, as $t \to \infty$, of (2.2).

Let $\lambda_1(\underset{\sim}{u}) \geq \lambda_2(\underset{\sim}{u}) \geq \dots$ be the eigenvalues of $\Lambda_{\underset{\sim}{u}}$, and $\underset{\sim}{\varphi}_1, \underset{\sim}{\varphi}_2 \cdots \underset{\sim}{\varphi}_k$ solutions of (2.1) for that $\underset{\sim}{u}$. Then

$$\text{(A3)} \qquad \lim_{t\to\infty} \frac{1}{t} \log \|\underset{\sim}{\varphi}_1 \wedge \cdots \wedge \underset{\sim}{\varphi}_k\| \quad ,$$

if it exists, is at most $\lambda_1(\underset{\sim}{u}) + \cdots + \lambda_k(\underset{\sim}{u})$, and equality holds for some choices of $\underset{\sim}{\varphi}_1, \dots, \underset{\sim}{\varphi}_k$.

The above statements are independent of measure. However, if we consider $L^2(\Omega, \mathbb{R}^n)$ as a measure space, we can also make statements about the existence of the limits (A1)-(A3). Our assumptions imply that the time evolution of (1) maps the set of initial conditions in K , after any finite time, to a compact subset $K(t) \subset L^2(\Omega, \mathbb{R}^n)$. Therefore, the solutions of (1.1) which take their values in K at time zero tend to a compact set $K = \bigcap_{t>0} K(t)$ when $t \to \infty$, and K is invariant under time evolution. It follows from the Markov-Kakutani fixed point theorem (see Dunford-Schwartz [7] I p.456) that there is at least one probability measure ρ with support in K which is invariant under time evolution, and we may assume that ρ is ergodic. (In general there will be many ergodic measures with support in K). Also the derivative $df^t_{\underset{\sim}{u}}$ is a compact linear operator on $L^2(\Omega,\mathbb{R}^n)$ which depends continuously on $\underset{\sim}{u}$. These conditions are sufficient to apply the multiplicative ergodic theorem. (This theorem was proved by Oseledec [22] for finite dimensional matrices; it extends to compact operators. as proved in Ruelle [24] and Mañé [21]). The theorem insures that, for almost all $\underset{\sim}{u}$ (with respect to ρ), and all $\underset{\sim}{\varphi}$, the limits (A1)-(A3) exist. Since ρ is ergodic, these limits are independent of $\underset{\sim}{u}$, but dependent on ρ .

If the time evolution defined by (1.1) has sensitive dependence on initial conditions, it actually produces information in the information-theoretic sense. The average amount of information $h(\rho)$ produced per unit time is the Kolmogorov-Sinai invariant, or entropy. At least for finite dimensional systems, it can be shown [23] that

(A4) $$h(\rho) < \text{sum of the positive characteristic exponents}$$

(There are important cases where equality holds. See in particular Bowen and Ruelle [2]). Assume that (A4) holds and let $w(x)$ be an upper bound to the largest eigenvalue of $\underset{\sim}{W} = \frac{1}{2}(dF+(dF)^*)$ as in Section 3. Then, since (A3) achieves its supremum $\sum_{i=1}^{k} \lambda_i(\rho)$, it follows from Lemma 1 that

(A5) $$\lambda_1(\rho)+\cdots+\lambda_k(\rho) \leq \lim_{t\to\infty} \frac{1}{T}\int_0^T dt\,(a_1+\cdots+a_k) = \int\rho(d\underset{\sim}{u})(a_1+\cdots+a_k)$$

where the a_j are as in Section 3. (Remember that w and therefore the a_j

depend on the time. By the ergodic theorem, the time average is replaced by an average over $\underset{\sim}{u} = \underset{\sim}{u}(0))$. Then the upper bounds obtained earlier for $h(u,t)$ apply also to $h(\rho)$, and these upper bounds are independent of ρ . We therefore obtain bounds on

$$h(K) = \sup_{\rho} h(\rho)$$

where the sup is taken over all ergodic measures with support in K . This sup is the <u>topological</u> entropy of K .

Because the compact set K is invariant under the maps f^t , and the derivatives $df^t_{\underset{\sim}{u}}$ are compact operators, it follows that K has finite Hausdorff dimension $\dim_H K$. A result of Ledrappier [18], based on earlier work by Frederikson, Kaplan and Yorke [11] and Douady and Oesterlé [6], yields the estimate

$$\text{(A6)} \qquad \dim_H K \leq \sup_{\rho} \max\{s : \tilde{c}(\rho,s) \geq 0\} \quad .$$

Here $\tilde{c}(\rho,k) = \sum_{i=1}^{k} \lambda_i(\rho)$, and $\tilde{c}$ interpolates linearly for non-integer values of the argument. From (A5), we see that our earlier estimates again apply to get bounds on $\dim_H K$. The estimate obtained for $\dim_H K$ is clearly also an upper bound for the number of non-negative characteristic exponents (for any ρ).

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