

Global Dynamics of Particles Driven by a Nonlinear Reaction-Diffusion Equation

During the pre-history of the academic lives of most people attending this workshop, Yasumasa Nishiura was producing global bifurcation diagrams, examining spectral information for singular systems, and discovering interesting dynamics. The first author had the privilege of meeting him during those early years and forever being influenced by his clear understanding and beautifully drawn pictures (on transparencies). His more recent excursion into and elucidation of shadow systems and behavior of solutions and coherent structures away from equilibrium states has also influenced our outlook. This paper, using spectral theory for singularly perturbed parabolic equations to understand temporal persistence of coherent structures clearly reflects some of those influences. This note is dedicated to our friend and colleague, Yasumasa Nishiura, on the occasion of his sixtieth birthday.

By

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Abstract

We demonstrate the existence of spatially localized solutions to a nonlinear heat equation which maintain their qualitative shape for all positive and negative time, being asymptotic in both directions of time to stationary peak-like solutions to the corresponding semilinear elliptic equation on a bounded smooth domain. This is accomplished by first producing a new global invariant manifold result for semiflows in Banach space. The main hypothesis for this abstract result is the existence of approximately invariant manifolds which are approximately normally hyperbolic. This theorem may be used in many other settings where good approximations to dynamically coherent structures are available.

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§ 1. Introduction

Starting with the work of Ni and Takagi [NT1], [NT2], and [NT3], many authors have discussed peak-like stationary states (particles) for the following nonlinear reaction-diffusion equation with small diffusion parameter $0 < \varepsilon \ll 1$

$$(1.1) \quad \begin{cases} u_t = \varepsilon^2 \Delta u - u + f(u), & x \in \Omega \\ \frac{\partial u}{\partial N} = 0, & x \in \partial\Omega. \end{cases}$$

Here Ω is a smoothly bounded domain in $\mathbb{R}^n$, N is the outward unit normal vector to $\partial\Omega$, and the nonlinearity f is smooth and is such that there is a non-degenerate positive radially symmetric ground state of the corresponding rescaled elliptic problem on $\mathbb{R}^n$.

These particular solutions, called least energy states, are almost zero on most of the domain but have a single sharp peak (spike) at a particular point on the boundary. As is suggested by the appellation, the approach taken was first variational, using constrained optimization, and then employing a refined analysis of the critical point, which showed that the profile of such a peaked solution is roughly given by a translation of the rescaled ground state w of the elliptic equation

$$(1.2) \quad \begin{cases} \Delta w - w + f(w) = 0, & y \in \mathbb{R}^n, \\ w(0) = \max w(y), & w > 0, \\ w(y) \rightarrow 0, & y \rightarrow \infty. \end{cases}$$

It is useful to think of the case $f(u) = u^p$ for some $p \in (1, p^*)$ where $p^* = \frac{n+2}{n-2}$ for $n \geq 3$ and $p^* = \infty$ when $n = 2$, even though more general nonlinearities are considered here. Note that the energy of a stationary state is then given by

$$E(u) \equiv \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + \frac{u^2}{2} - \frac{u^{p+1}}{p+1} \right).$$

In this pure power case one can consider the quadratic functional

$$Q(v) \equiv \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla v|^2 + \frac{v^2}{2} \right)$$

and minimize it on the manifold

$$\mathcal{H} \equiv \{v : \int_{\Omega} v^{p+1} = 1\}.$$

The constraint introduces a Lagrange multiplier and a scaling of the minimizer, $u = \alpha v$, gives the desired solution.

We can also see that the peak should have its maximum exactly on $\partial\Omega$, located close to where $\partial\Omega$ has greatest mean curvature. To explain this, note that Q has two

parts, bulk and interfacial. In minimizing Q among states in $\mathcal{H}$ one can make the bulk energy arbitrarily close to zero by shrinking the support of functions while staying in $\mathcal{H}$ (possible because $p > 1$) but at a cost in having a larger interfacial energy. These are balanced at the ε -scaled ground state profile. That profile is almost zero except for an ε -small region inside which the spike occurs. The bulk energy is roughly proportional to the volume of the region in Ω where the spike is ‘supported’ and essentially remains the same regardless of the location of the peak in the interior of the domain. However, the interfacial energy is roughly proportional to the surface area of this region *lying within* Ω and furthermore, the support of the spike can be reduced at no interfacial energy cost by having the spike on $\partial\Omega$. Thus, the energy is minimized by having this region be spherical, and further by the center being on $\partial\Omega$. A final small reduction is achieved, when ε is small, by having the center (the location of the peak) on the boundary at the point where the mean curvature is greatest, since at such a point we maximize the use of $\partial\Omega$ in bounding the part of the peak region that lies in Ω . The analysis performed by Ni and Takagi makes rigorous this reasoning.

The key point to note is that, when ε is small, the scaled ground state, translated to the boundary, is a very good approximation to the stationary solution, and that moving it along the boundary changes the energy slightly, according to the mean curvature of the boundary.

The main result presented here, which is given in complete detail in [BLZ5], takes this key idea and instead of seeking only stationary states, places a particle (peak state) at any point of $\partial\Omega$ and allows it to crawl along the boundary, maintaining its rough shape, as it seeks a location that minimizes Q , at least locally. In fact we construct a solution to (1.1) which has the form of an ε -scaled ground state centered at a point moving on $\partial\Omega$, and furthermore, the solution exists globally in time, forward and *backward*.

Of course, a translated copy of an ε -scaled ground state does not satisfy the boundary condition on $\partial\Omega$ and so some small modification is needed so that the boundary condition is satisfied. On the other hand, this initial state must be very special for it to produce a solution that exists backward in time. Our approach is to realize the existence of such initial states (and hence global in time solutions) by establishing the existence of a global invariant manifold for (1.1) as a graph over (and very close to) the manifold, M_ε , (in function space) that is obtained by translating the ε -scaled ground state to each point of $\partial\Omega$ and modifying to satisfy the boundary condition. This image of $\partial\Omega$ in function space is a smooth manifold (as smooth as $\partial\Omega$) and it is almost invariant under (1.1); indeed, each point of it is almost stationary. Also, it is almost *normally hyperbolic* in the following sense (to be made precise later): The operator obtained by linearizing the right hand side of (1.1) at each point of the manifold has a codimensional- n eigenspace corresponding to negative spectrum (bounded away from

0), a one-dimensional eigenspace corresponding to a large positive eigenvalue, and a complementary $(n - 1)$ -dimensional eigenspace that is almost the tangent space of the manifold and which corresponds to eigenvalues that are close to zero.

The outcome is that there must exist a manifold $\tilde{M}_\varepsilon$, that is very close to M_ε which is truly invariant under (1.1). Examples where approximately invariant manifolds are constructed for singularly perturbed parabolic equations, in some cases leading to truly invariant manifolds, may be found in [FH, CP1, CP2, ABF, BX1, BX2, AF, BFu, Wei], for instance.

The idea described in the above paragraph is abstract and rather general. In the next section we present the general theorem for semiflows in Banach space which essentially states that if a C^1 semiflow has a compact manifold that is approximately invariant and approximately normally hyperbolic, then it has nearby a truly normally hyperbolic invariant manifold.

The abstract result is then applied to our PDE to obtain the following theorem:

Theorem 1.1. *Under the assumptions mentioned above, for any sufficiently small $\varepsilon > 0$, there exists a smooth mapping $\Psi_\varepsilon : \partial\Omega \rightarrow W^{2,2}(\Omega)$ such that*

1. *For any $q \in (n, \infty)$, there exists $C > 0$ independent of $p \in \partial\Omega$ and sufficiently small $\varepsilon > 0$ such that*

$$\begin{aligned} |\Psi_\varepsilon(p) - w(\frac{\cdot - p}{\varepsilon})|_{C^0((\partial\Omega, W^{2,q}(\Omega)))} &\leq C\varepsilon \\ |\Psi_\varepsilon(p) - w(\frac{\cdot - p}{\varepsilon})|_{C^1((\partial\Omega, W^{2,q}(\Omega)))} &\rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0. \end{aligned}$$

2. *There exists a unique $\tilde{p} \in \partial\Omega$ such that $\max_{x \in \bar{\Omega}} \Psi_\varepsilon(p)(x) = \Psi_\varepsilon(p)(\tilde{p})$. Moreover $|p - \tilde{p}| < C\varepsilon^2$ for some $C > 0$ independent of $0 < \varepsilon < 1$.*
3. *$M_\varepsilon^* \equiv \Psi_\varepsilon(\partial\Omega)$ is a normally hyperbolic invariant manifold of the flow generated by equation (1.1).*
4. *Equation (1.1) induces a vector field $Y_\varepsilon(p)$ on $\partial\Omega$ that satisfies*

$$|Y_\varepsilon(p) - c\varepsilon^3 \nabla \kappa(p)| \leq C\varepsilon^4$$

for some $C > 0$ independent of $p \in T_p \partial\Omega$ and sufficiently small $\varepsilon > 0$ and $c > 0$ determined only by w , where $\kappa(p) = H(p) \cdot N(p)$ and $H(p)$ is the mean curvature vector of $\partial\Omega$.

§ 2. Semiflows in Banach Space

Let X be a Banach space and let T be a C^1 map from X into X . We do not assume invertibility and so the results will apply to semi-dynamical systems such as the time- t map of the solution operator for a nonlinear parabolic partial differential equation.

Suppose that there exists a smooth manifold, $\tilde{M}$, embedded in X , which is approximately invariant with respect to T , that is, for some small $\delta > 0$

$$T(\tilde{M}) \subset B(\tilde{M}, \delta)$$

and

$$\tilde{M} \subset B(T(\tilde{M}), \delta),$$

where $B(\tilde{M}, \delta) = \{x \in X : \text{dist}(x, \tilde{M}) < \delta\}$ is a δ neighborhood of $\tilde{M}$.

Our general results include the cases where the manifold is immersed, rather than embedded in X but here we only discuss the most straightforward situation of embedded manifolds.

The questions which are addressed here concern the existence of a true invariant manifold for T and the qualitative behavior of the orbits near this invariant manifold. In general there will be no true invariant manifold for T even in finite-dimensional space. In fact our results are new even in the finite-dimensional setting. In order to guarantee the existence of a true invariant manifold, a nondegeneracy condition on the approximately invariant manifold is necessary. This condition is *approximate normal hyperbolicity*. The condition gives, for each $m \in \tilde{M}$, a decomposition $X = X_m^c \oplus X_m^u \oplus X_m^s$, with X_m^c an approximation of the tangent space to $\tilde{M}$ at m and such that

- (a) This splitting is approximately invariant under the linearized map, DT ,
- (b) $DT(m)|_{X_m^u}$ expands and does so to a greater degree than does $DT(m)|_{X_m^c}$ while $DT(m)|_{X_m^s}$ contracts and does so to a greater degree than does $DT(m)|_{X_m^c}$,
- (c) The splitting varies in a Lipschitz continuous way and the angles between the subspaces is uniformly bounded below.

The superscripts c, u and s stand for “center,” “unstable,” and “stable,” respectively.

Heuristically, our main results may be summarized by

Theorem 2.1.

Suppose that $\tilde{M}$ is a C^1 manifold which is approximately invariant and approximately normally hyperbolic with respect to T , the approximation being sufficiently good and the “twisting” of $\tilde{M}$ being uniformly bounded, then

- (1) *Existence:* T has a true C^1 normally hyperbolic invariant manifold M near $\tilde{M}$.
- (2) *Smoothness:* If T is C^k and a “spectral gap” condition holds, then M is C^k .
- (3) *Stable and Unstable Manifolds:* There is a stable manifold $W^s(M)$ and an unstable manifold $W^u(M)$ of T at M .

(4) *Invariant Foliations: Both $W^s(M)$ and $W^u(M)$ are foliated by invariant foliations:*

$$W^s(M) = \cup_{m \in M} W_m^{ss} \quad \text{and} \quad W^u(M) = \cup_{m \in M} W_m^{uu},$$

where leaves W_m^{ss} and W_m^{uu} are C^k submanifolds and are Hölder continuous in m .

(5) *Characterization of Foliations: For any $x, \tilde{x} \in W_m^{ss}$, $|T^n(\tilde{x}) - T^n(x)| \rightarrow 0$ exponentially, as $n \rightarrow +\infty$; For any $y, \tilde{y} \in W_m^{uu}$, $|T^n(\tilde{y}) - T^n(y)| \rightarrow 0$ exponentially, as $n \rightarrow -\infty$.*

(6) *Semiflow: If $\tilde{M}$ is an approximately invariant manifold of time- t_0 map T^{t_0} of a semiflow at $t_0 > 0$, then the semiflow T^t has a normally hyperbolic invariant manifold.*

Remarks: We do not assume that M is compact or finite-dimensional. Also, M is not necessarily an embedded manifold, but may be an immersed manifold. We assume that the immersed manifold M does not twist very much locally, and DT has a certain uniform continuity in a neighborhood of M . Note that in item 5, above, it is part of the result that T^{-1} exists on the unstable manifold.

In the case of a C^2 manifold, the conditions in the theorem can be more easily described:

Assume a.) M is a C^2 manifold embedded into a Banach space so that there exists $r > 0$ and for any $x \in M$, the r -neighborhood of x in M can be written as the graph of a mapping with C^2 bounds uniform in x . b.) the semiflow T^t has finite C^2 norm on $B(M, r)$ for t on any finite interval. c.) The projections associated to the approximately normal hyperbolic splitting are uniformly bounded and have a finite Lipschitz constant, where the former means that the angle between the splitting is uniformly bounded from below and the latter means the splitting changes in a Lipschitz fashion with respect to the base point. Roughly, let $\eta > 0$ measure the error of the approximate invariance of M under T^{t_0} for some $t_0 > 0$ and $\sigma > 0$ measure the error of the approximate invariance of the splitting under DT^{t_0} . There exist (i) σ_0 depending on the upper bound for the norms of the projection operators in the splitting, the C^2 bounds of T^{t_0} and the contracting rates of DT^{t_0} in the stable direction, expanding rates in the unstable direction, and its forward and backward bounds in the tangent direction and (ii) η_0 , depending, in addition, on the C^2 bounds on both the geometry and the embedding of M , and the Lipschitz bounds of the splitting such that if $\sigma < \sigma_0$ and $\eta < \eta_0$, then the conclusions of the above theorem hold. The way in which these constants depend upon the parameters is given in [BLZ5], for instance in Theorem 4.2 and the lemmas that give its proof.

The above result can be viewed as an extension of [BLZ1] and [BLZ2] where perturbations of semiflows are considered. Those two papers are themselves extensions to

semiflows to the fundamental results of Fenichel [F1, F2, F3] and of Hirsch, Pugh and Shub [HPS] on persistence of invariant manifolds for flows (or homeomorphisms). Those papers have formed the basis for geometric singular perturbation theory [JK, CKRTJ2] and have been crucial in the analysis of many equations arising in the applied sciences, such as the FitzHugh-Nagumo equations [CKRTJ] and the equations of gas dynamics [Sch], for instance.

The results presented here likewise should be applicable in many situations where one may easily find manifolds of approximately stationary states or coherent structures that change slowly in time. This is especially common in systems of singularly perturbed nonlinear parabolic PDEs such as the above example, the Cahn-Hilliard equation, and for the Gierer-Meinhardt or the Gray-Scott systems, where distinctive patterned states are found as the singular parameter approaches zero.

§ 3. Some ideas behind the proofs:

We use an approach due to Hadamard [H] in which any Lipschitz graph is transported by the map or semiflow, producing a new graph and the operation is a contraction on the space of Lipschitz graphs.

We actually get a **Center-Stable Manifold** W^{cs} and a **Center-Unstable Manifold** W^{cu} and intersect them to get $\tilde{M}$.

CENTER-UNSTABLE MANIFOLD:

Let

$$M^u \equiv \{m + x^u : m \in M, x^u \in X_m^u, |x^u| < \delta\}.$$

This is approximately stably normally hyperbolic and is approximately “overflowing” invariant.

Let Γ_u be the set of μ -Lipschitz graphs over M^u for some small μ . As T maps each member of Γ_u forward, the graph is “stretched tangentially” and “compressed normally”. Thus, it is mapped by T into Γ_u and, furthermore, the mapping is a contraction in the sup norm. The fixed graph is W^{cu} . The details involve the use of local coordinate representations of graphs and the expression of the approximate normal hyperbolicity of the mapping in local coordinates. This is fairly messy but the essence of the proof is what is stated above.

CENTER-STABLE MANIFOLD:

For W^{cs} , we consider Γ_s of Lipschitz graphs over M^s , the corresponding stable bundle. Since T shrinks these graphs tangentially and expands normally, Γ_s is not preserved under T . One would like to take the inverse image of each member of Γ under T , which

would again be a contraction. However, T is not a homomorphism (e.g. the time-1 map of a parabolic flow), and so it seems that one cannot find a preimage of the graph.

What we show is the following

Lemma Let $h \in \Gamma_s$. For each point $m + x^s \in M^s$, with $|x^s|$ small, there is a point $x^u \in X_m^u$ such that $T(m + x^s + x^u) \in \text{graph}(h)$.

This is proved using a contraction argument but the essential idea is that the unstable fiber $m + x^s + X_m^u$ is stretched by T in the unstable direction while in the transverse direction it is held close to M and so the image intersects $\text{gr}(h)$ at a single point, y say. Thus, for each $m + x^s \in M^s$ there is a point $x^u = x^u(m + x^s) \in X_m^u$ with $T(m + x^s + x^u) = y \in \text{graph}(h)$.

This provides a graph $\text{gr}(\tilde{h})$ over M^s that maps *into* $\text{gr}(h)$. Using the approximate normal hyperbolicity, we show that $\tilde{h} \in \Gamma_s$ and that the mapping $h \rightarrow \tilde{h}$ is a contraction, and so has a fixed point $h_0 \in \Gamma_s$. This fixed graph is W^{cs} , the center-stable manifold. Details for the above are found in [BLZ5], Theorem 4.2, in particular.

Since the bundles X^s and X^u are transverse, W^{cs} and W^{cu} intersect transversally in an invariant manifold $\tilde{M}$.

§ 4. The application

We build an approximately invariant approximately normally hyperbolic manifold by taking the rescaled radially symmetric ground state w satisfying

$$\begin{cases} \Delta w + f(w) = 0, & y \in \mathbb{R}^n, \\ w(0) = \max w(y), & w > 0, \\ w(y) \rightarrow 0, & |y| \rightarrow \infty. \end{cases}$$

It is assumed that f is such that w is unique and nondegenerate (see [BLP]).

With $L_0 \equiv \Delta + f'(w) : W^{2,q}(\mathbb{R}^n) \rightarrow L^q(\mathbb{R}^n)$, its spectrum satisfies $\sigma(L_0) \cap (-b, \infty) = \{\lambda_1, 0\}$, for some $b > 0$; $\lambda_1 > 0$ is the principle eigenvalue, and the eigenspace of $\lambda = 0$ is spanned by

$$\left\{ \frac{\partial w}{\partial y_j} : j = 1, 2, \dots, n \right\}.$$

For $u \in W^{2,q}$ define

$$|u|_{k,\varepsilon}^q = \sum_{i=0}^k \varepsilon^{qi-n} \sum_{|\alpha|=i} |\partial^\alpha u|_{L^q(\Omega)}^q.$$

The phase space will be taken as $X = (W^{2,q}(\Omega), |\cdot|_{0,\varepsilon})$. Let $L_* = \varepsilon^2 \Delta + f'(0)$ with the domain

$$D(L_*) = \{u \in H^2(\Omega) \mid \frac{\partial u}{\partial N}(x) = 0, x \in \partial\Omega\}.$$

Here we skip some details to show that the conditions of the abstract theorem hold in the hope of giving the general ideas.

For any $p \in \partial\Omega$, let

$$\tilde{w}_{\varepsilon,p}(x) = w\left(\frac{x-p}{\varepsilon}\right).$$

Since $\tilde{w}_{\varepsilon,p}$ does not satisfy the boundary condition, it is modified as follows:

Given any $v : \partial\Omega \rightarrow R$, let h be the solution of

$$\begin{cases} \varepsilon^2 \Delta h + f'(0)h = 0, & x \in \Omega, \\ \frac{\partial h}{\partial N} = v, & x \in \partial\Omega. \end{cases}$$

Define a linear operator Bc by $Bc(v) = h$. For $p \in \partial\Omega$, let

$$W_{\varepsilon,p} = \tilde{w}_{\varepsilon,p} - Bc\left(\frac{\partial \tilde{w}_{\varepsilon,p}}{\partial N}\right).$$

Thus, we may define a smooth imbedding $\psi_\varepsilon : \partial\Omega \rightarrow L^2(\Omega)$ by

$$\psi_\varepsilon(p) \equiv W_{\varepsilon,p}$$

and the approximate invariant manifold

$$M_\varepsilon = \psi_\varepsilon(\partial\Omega).$$

The boundary correction $Bc(\frac{\partial \tilde{w}_{\varepsilon,p}}{\partial N})$ is of order $O(\varepsilon)$ in terms of $|\cdot|_{k,\varepsilon}$ for any $k \geq 0$, up to a restriction from the regularity of the boundary and f . In fact, using elliptic estimates and the trace theorem, we have, for $k \geq 0$,

$$|Bc(v)|_{k+1,\varepsilon}^q \leq C \sum_{j=0}^k \varepsilon^{3+qj-n} |v|_{W^{j,q}(\partial\Omega)}^q.$$

In our case, because $\tilde{w}_{\varepsilon,p}$ is exponentially localized with spatial scale ε and because it is radially symmetric, for $x \in \partial\Omega$ with $|x-p| = O(\varepsilon)$, the angle between $\nabla \tilde{w}_{\varepsilon,p}(x)$ and the normal $N(x)$ is $O(\varepsilon)$. Thus,

$$\left| \frac{\partial \tilde{w}_{\varepsilon,p}}{\partial N} \right|_{W_{k,\varepsilon}^q(\partial\Omega)} = O(\varepsilon),$$

and the claim above follows. This implies

$$|\psi_\varepsilon(p) - \tilde{w}_{\varepsilon,p}|_{k+1,\varepsilon} = O(\varepsilon),$$

and so $\psi_\varepsilon(p)$ satisfies the boundary condition and

$$|(\varepsilon^2 \Delta - 1)\psi_\varepsilon(p) + f(\psi_\varepsilon(p))|_{k-1,\varepsilon} = |f(\psi_\varepsilon(p)) - f(\tilde{w}_{\varepsilon,p})|_{k-1,\varepsilon} = O(\varepsilon),$$

i.e., it is approximately stationary (and so approximately invariant) under the time- t_0 solution operator of the nonlinear parabolic equation, with error $O(\varepsilon)$.

Let $v_1 > 0$ be the first eigenfunction, corresponding to the eigenvalue λ_1 , of the linearized operator L_0 .

For any $p \in \partial\Omega$, define

$$\tilde{v}_{\varepsilon,p}(x) = v_1\left(\frac{x-p}{\varepsilon}\right), \quad V_\varepsilon(p) = \tilde{v}_{\varepsilon,p} - Bc\left(\frac{\partial}{\partial N}\tilde{v}_{\varepsilon,p}\right),$$

and

$$X_{\varepsilon,p}^u = \text{span}\{V_\varepsilon\}, \quad X_{\varepsilon,p}^c = T_{\psi_\varepsilon(p)}M_\varepsilon, \quad X_{\varepsilon,p}^s = (X_{\varepsilon,p}^c \oplus X_{\varepsilon,p}^u)^\perp,$$

where the L^2 orthogonal complement defining X^s is taken in X . Then one can show that this splitting is approximately invariant under the linearized time- t_0 solution operator at any point of M_ε , with error $O(\varepsilon)$.

The constructed manifold M_ε is approximately invariant and approximately normally hyperbolic in the sense of the abstract results, provided ε is sufficiently small.

Applying Theorem 3.1 we obtain a truly invariant manifold $\tilde{M}_\varepsilon$ in a small $W^{k,q} \subset C(\bar{\Omega})$ neighborhood of M_ε , which therefore consists of spike-like functions.

Finally, one can compute the vector field on $\tilde{M}_\varepsilon$ induced by the equation, obtaining a dynamical system on $\partial\Omega$ for the evolving location of the maximum of the spike. Details for the above are found in [BLZ5], section 7.

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