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A BU THESIS LATEX TEMPLATE

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*Facilis descensus Averni;
Noctes atque dies patet atri janua Ditis;
Sed revocare gradum, superasque evadere ad auras,
Hoc opus, hic labor est.* Virgil (from Don's thesis!)

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[This is where the acknowledgments go...]

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ABSTRACT

[This is where the text for the abstract will go]

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List of Abbreviations

| | | |
|------|-------|----------------------------|
| FPUT | | Fermi-Pasta-Ulam-Tsingou |
| mKdV | | modified Korteweg-De Vries |

Chapter 1

Background Material

1.1 Fenichel Theory

(Wiggins, 1994)

$$\dot{x} = f(x), \quad x \in \mathbb{R}^n \quad (1.1)$$

Definition 1. Let $\overline{M} = M \cup \partial M$ be a compact, connected C^r manifold with boundary contained in \mathbb{R}^n . Then \overline{M} is said to be overflowing invariant under eq. (1.1) if for every $p \in \overline{M}$, $\phi_t(p) \in \overline{M}$ for all $t \leq 0$ and the vector field eq. (1.1) is pointing strictly outward on ∂M .

Theorem 1. Suppose $\dot{x} = f(x)$ is a C^r vector field on \mathbb{R}^n , $r \geq 1$. Let $\overline{M} = M \cup \partial M$ be a C^r , compact connected manifold with boundary overflowing invariant under the vector field $f(x)$. Suppose $\nu^s(p) < 1$, $\lambda^u(p) < 1$, and $\sigma^s(p) < \frac{1}{r}$ for all $p \in M$. Then there exists a C^r overflowing invariant manifold $W^u(\overline{M})$ containing \overline{M} and tangent to $h_u(N_\epsilon'^u)$ along \overline{M} with trajectories in $W^u(\overline{M})$ approaching \overline{M} as $t \rightarrow -\infty$.

Theorem 2. Suppose $\dot{x} = f(x)$ is a C^r vector field on \mathbb{R}^n , $r \geq 1$. Let $\overline{M} = M \cup \partial M$ be a C^r compact connected manifold with boundary, overflowing invariant under the vector field $f(x)$. Suppose $\lambda^u(p) < 1$, $\sigma^{cu}(p) < 1$, and $\sigma^{su}(p) < 1$ for every $p \in \overline{M}_1$. Then there exists a $n - (s + u)$ -parameter family $\mathcal{F}^u = \cup_{p \in M} f^u(p)$ of u -dimensional surfaces $f^u(p)$ (with boundary) such that the following hold:

1. \mathcal{F}^u is a negatively invariant family, i.e., $\phi_{-t}(f^u(p)) = f^u(\phi_{-t}(p))$ for any $t \geq 0$ and $p \in M$.
2. The u -dimensional surfaces $f^u(p)$ are C^r .
3. $f^u(p)$ is tangent to $h_u(N_p'^u)$ at p .

4. *There exists $C_u, \lambda_u > 0$ such that if $q \in f^u(p)$, then*

$$|\phi_{-t}(q) - \phi_{-t}(p)| < C_u e^{-\lambda_u t}$$

for any $t \geq 0$.

5. *Suppose $q \in f^u(p)$ and $q' \in f^u(p')$. Then*

$$\frac{|\phi_{-t}(q) - \phi_{-t}(p)|}{|\phi_{-t}(q') - \phi_{-t}(p)|} \rightarrow 0 \quad \text{as } t \rightarrow \infty$$

unless $p = p'$.

6. *$f^u(p) \cap f^u(p') = \emptyset$, unless $p = p'$.*

7. *If the hypotheses of the unstable manifold theorem hold, i.e., if additionally $\nu^s(p) < 1$ and $\sigma^s(p) < \frac{1}{r}$ for every $p \in \overline{M}_1$, then the u -dimensional surfaces $f^u(p)$ are C^r with respect to the basepoint p .*

8. $\mathcal{F}^u = W_{\text{loc}}^u(M)$.

Chapter 2

Existence of Kink-Like Traveling Wave Solutions

2.1 Introduction

The goal of this chapter is to show the existence of the travelling wave solution for the FPUT lattice and describe its profile. From formal calculations and the numerical experiments carried out in (Pace et al., 2019), one expects that the travelling wave solution has a profile given by the kink solution to the mKdV; that is, for $\phi(\xi) = \frac{1}{\sqrt{2}} \tanh(\xi/\sqrt{2})$ we expect to have a travelling wave solution u such that

$$u_n(t) = \epsilon \phi(\epsilon(n + ct)) + \mathcal{O}(\epsilon^3) \quad (2.1)$$

when c is slightly smaller than $V''(0) = 1$.

One would expect that methods used to find the soliton-like solution for the FPUT can also be applied to this case. Notably Friesecke and Pego showed in (Friesecke and Pego, 1999) that there exists a solitary wave solution whose profile is described by the KdV soliton using a fixed-point argument. The argument relies on creating a map from $H^1(\mathbb{R})$ to itself using Fourier multipliers such that the fixed point of the map is the profile of the solitary wave. However, this argument does not extend to our case since the function ϕ is not in a Sobolev space and its Fourier transform is defined only in a distributional sense. Due to this problem, we neglect the functional approach and focus on techniques from bifurcation theory.

One common technique for constructing travelling wave solutions to PDEs is by using the center manifold theorem. For PDEs of one spatial and one temporal variable, the strategy is to assume that the solution is a travelling wave (i.e. of the form $f(x - ct)$) to eliminate the derivative with respect to t and reduce the problem to an ODE with respect to the spatial variable x . Finding bounded solutions of this ODE then results in travelling wave solutions of the PDE. The center manifold is an important tool for finding these solutions since (1) it is finite-dimensional, (2) can typically be approximated by Taylor series up to arbitrary order, and (3) contains all bounded solution. If a linear operator has an eigenvalue pass through the line $\{\lambda \in \mathbb{C} : \Re \lambda = 0\}$ as a parameter μ varies, then one typically has a center manifold containing small bounded parameterized by μ . Such a construction was carried out in (Iooss, 2000), in which the existence of several travelling wave solutions were proved. The bifurcation parameter in this paper was given in part by the wave speed. In fact, [Thm. 5](Iooss, 2000) shows the existence of a heteroclinic orbit on the center manifold when c is slightly smaller than 1. This heteroclinic orbit corresponds to the kink-like solution of the FPUT we are interested in. But no description of its wave profile was given, so obtaining an estimate of the form in eq. (2.1) is still an open problem.

Our argument for getting such an estimate will proceed as follows. We first follow the procedure in (Iooss, 2000) to construct the center manifold parameterized by ϵ , making sure to explicitly compute the dynamics on the center manifold. Making a suitable change of variables, we look for small-amplitude, long-wavelength solutions for the FPUT on the center manifold and show that formally setting $\epsilon = 0$ gives a solution related to the kink solution ϕ . Next we apply results from Fenichel theory to show that this solution persists for $\epsilon > 0$. Lastly we convert our results back to the original formulation of the FPUT lattice and prove an estimate of the form eq. (2.1).

2.2 Construction of Center Manifold

We follow the construction of the center manifold carried out in (Iooss, 2000). Recall that the equations for the FPUT lattice are given by

$$\ddot{x}_n = V'(x_{n+1} - x_n) - V'(x_n - x_{n-1}), \quad n \in \mathbb{Z}. \quad (2.2)$$

We assume that $V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4 + \mathcal{O}(x^5)$ near $x = 0$. We make the ansatz that

$$x_n(\tilde{t}) = x(n - c\tilde{t}), \quad (2.3)$$

where the $x(t)$ on the right is a function from \mathbb{R} to \mathbb{R} . Hence $x(t)$ must satisfy the advance-delay differential equation

$$\ddot{x}(t) = \mu \left(V'(x(t+1) - x(t)) - V'(x(t) - x(t-1)) \right) \quad (2.4)$$

where $\mu = c^{-2}$. Instead of working directly with eq. (2.4), we rewrite the equation as a first-order differential equation in a Banach space. Equation (2.4) cannot be written as a differential equation in a finite-dimensional phase space, and so we use a Banach space to represent a “slice” of the function on the interval $[t-1, t+1]$ for $t \in \mathbb{R}$. We introduce a new variable $v \in [-1, 1]$ and functions $X(t, v) = x(t+v)$. We use the notation $\xi(t) = \dot{x}(t)$, $\delta^1 X(t, v) = X(t, 1)$, and $\delta^{-1} X(t, v) = X(t, -1)$. Then letting $U(t) = (x(t), \xi(t), X(t, v))^T$ represent our solution, eq. (2.4) can be written as follows:

$$\partial_t U = L_\mu U + M_\mu(U) \quad (2.5)$$

where L_μ is the linear operator

$$L_\mu = \begin{pmatrix} 0 & 1 & 0 \\ -2\mu & 0 & \mu(\delta^1 + \delta^{-1}) \\ 0 & 0 & \partial_v \end{pmatrix} \quad (2.6)$$

and

$$M_\mu(U) = \mu(0, g(\delta^1 X - x) - g(x - \delta^{-1} X), 0)^T \quad (2.7)$$

where we define $g(x) = V'(x) - x$. We will also require that $X(t, 0) = x(t)$, so that $X(t, v) = x(t + v)$ and solutions of eq. (2.5) correspond with solutions of eq. (2.4). We introduce the following Banach spaces for U :

$$\begin{aligned} \mathbb{H} &= \mathbb{R}^2 \times C[-1, 1] \\ \mathbb{D} &= \{U \in \mathbb{R}^2 \times C^1[-1, 1] \mid X(0) = x\} \end{aligned} \quad (2.8)$$

where the spaces have the usual maximum norms. The operator L_μ is continuous from \mathbb{D} to \mathbb{H} . Assuming that $g \in C^4(I)$ where I is an open neighborhood around 0, we have $M_\mu \in C^4(\mathbb{D}, \mathbb{D})$.

Note that eq. (2.5) is not well-posed and solutions may not correspond with the requirement that $X(t, 0) = x(t)$. However, we can show that there is a center manifold which contains global solutions and lies in \mathbb{D} , and so we will be able to extract the travelling wave solutions that we are interested in.

As shown in (Iooss, 2000, Lem. 1), when $\mu = \mu_0 := 1$ (i.e. when $c = \sqrt{V''(0)} = 1$) the linear operator L_{μ_0} has a quadruple zero eigenvalue with the rest of the spectrum bounded uniformly away from the imaginary axis. This allows for the construction of a four-dimensional center manifold. This construction is not carried out explicitly in (Iooss, 2000), but it follows similarly to the calculations carried out in (Iooss and Kirchgässner, 2000) which relies on results in (Vanderbauwhede and Iooss, 1992).

The four-dimensional eigenspace for $\lambda = 0$ is spanned by the following generalized eigenfunctions:

$$\begin{aligned} \zeta_0 &= (1, 0, 1)^T & \zeta_1 &= (0, 1, v)^T \\ \zeta_2 &= (0, 0, \frac{1}{2}v^2)^T & \zeta_3 &= (0, 0, \frac{1}{6}v^3)^T \end{aligned} \quad (2.9)$$

which satisfy

$$\begin{aligned}
L_{\mu_0}\zeta_0 &= 0 \\
L_{\mu_0}\zeta_1 &= \zeta_0 \\
L_{\mu_0}\zeta_2 &= \zeta_1 \\
L_{\mu_0}\zeta_3 &= \zeta_2.
\end{aligned} \tag{2.10}$$

The spectral projection onto the eigenspace can be found using the Laurent expansion in $\mathcal{L}(\mathbb{H})$ near $\lambda = 0$

$$(\lambda\mathbf{I} - L_{\mu_0})^{-1} = \frac{D^3}{\lambda^4} + \frac{D^2}{\lambda^2} + \frac{D}{\lambda^2} + \frac{P}{\lambda} - \tilde{L}_{\mu_0}^{-1} + \lambda\tilde{L}_{\mu_0}^{-1} - \dots \tag{2.11}$$

where P is the spectral projection, $D = L_{\mu_0}P$, and $\tilde{L}_{\mu_0}^{-1}$ is the pseudo-inverse of L_{μ_0} on the subspace $(\mathbf{I} - P)\mathbb{H}$ (see (Kato, 2013)). The spectral projection satisfies

$$\begin{aligned}
PW &= ((PW)_x, (PW)_\xi, (PW)_X)^T \\
&= (PW)_x\zeta_0 + (DW)_x\zeta_1 + (D^2W)_x\zeta_2 + (D^3W)_x\zeta_3
\end{aligned} \tag{2.12}$$

The projection can be computed by finding the resolvent $(\lambda\mathbf{I} - L_\mu)^{-1}$ and then determining the residue of a meromorphic function. The resolvent operator is straightforward to compute. For $F = (f_0, f_1, F_2)^T \in \mathbb{H}$, we want to find $U = (x, \xi, X)^T \in \mathbb{D}$ such that

$$(\lambda\mathbf{I} - L_\mu)U = F. \tag{2.13}$$

The operator on the left-hand side when $N(\lambda; \mu) \neq 0$ where

$$N(\lambda; \mu) = -\lambda^2 + 2\mu(\cosh \lambda - 1) \tag{2.14}$$

and U is given by

$$x = -[N(\lambda; \mu)]^{-1}(\lambda f_0 + f_1 + \mu \tilde{f}_\lambda) \quad (2.15)$$

$$\xi = -[N(\lambda; \mu)]^{-1}([\lambda^2 + N(\lambda; \mu)]f_0 + \lambda f_1 + \mu \lambda \tilde{f}_\lambda) \quad (2.16)$$

$$X(v) = e^{\lambda v} x - \int_0^v e^{\lambda(v-s)} F_2(s) ds \quad (2.17)$$

with

$$\tilde{f}_\lambda = \int_0^1 [-e^{\lambda(1-s)} F_2(s) + e^{-\lambda(1-s)} F_2(-s)] ds. \quad (2.18)$$

Hence, the projection can be computed by standard techniques. For instance, note that

$$(PF)_x = \text{Res}((\lambda I - L_{\mu_0}^{-1} F)_x, 0) = \text{Res}(-[N(\lambda; \mu)]^{-1}(\lambda f_0 + f_1 + \mu \tilde{f}_\lambda), 0). \quad (2.19)$$

For fixed $F \in \mathbb{H}$, the last can be found by finding the residue of a meromorphic function in \mathbb{C} . Proceeding in this way, we can get

$$(PF)_x = \frac{2}{5} \left(f_0 - \int_0^1 [(1-s) - 5(1-s)^3][F_2(s) + F_2(-s)] ds \right) \quad (2.20)$$

$$(DF)_x = (PF)_\xi = \frac{2}{5} \left(f_1 - \int_0^1 [1 - 15(1-s)^2][F_2(s) - F_2(-s)] ds \right) \quad (2.21)$$

$$(D^2 F)_x = (DF)_\xi = -12 \left(f_0 - \int_0^1 (1-s)[F_2(s) + F_2(-s)] ds \right) \quad (2.22)$$

$$(D^3 F)_x = (D^2 F)_\xi = -12 \left(f_1 - \int_0^1 [F_2(s) - F_2(-s)] ds \right). \quad (2.23)$$

We denote by ζ_j^* the linear continuous forms on \mathbb{H} given for any $F \in \mathbb{H}$ by

$$\begin{aligned}\zeta_0^*(F) &= (PF)_x \\ \zeta_1^*(F) &= (DF)_x = \zeta_0^*(L_{\mu_0}F) \\ \zeta_2^*(F) &= (D^2F)_x \\ \zeta_3^*(F) &= (D^3F)_x\end{aligned}\tag{2.24}$$

and we have that

$$\zeta_k^*(\zeta_j) = \delta_{kj} \quad k, j = 0, 1, 2, 3\tag{2.25}$$

where δ_{kj} is the Kronecker delta.

At this point we could start to compute the four-dimensional center manifold parameterized by μ , but we can do a further simplification. Note that eq. (2.5) is invariant under

$$U \mapsto U + q\zeta_0, \quad \forall q \in \mathbb{R}\tag{2.26}$$

which corresponds to the shift invariance of eq. (2.4). This invariance allows us to reduce the center manifold to a three-dimensional manifold. We first decompose $U \in \mathbb{H}$ as follows:

$$U = W + q\zeta_0, \quad \zeta_0^*(W) = 0.\tag{2.27}$$

Denote by \mathbb{H}_1 to codimension-one subspace of \mathbb{H} where $\zeta_0^*(W) = 0$, and similarly define \mathbb{D}_1 . Then the system in eq. (2.5) becomes

$$\frac{dq}{dt} = \zeta_0^*(L_\mu W) = \zeta_0^*(L_{\mu_0} W) = \zeta_1^*(W)\tag{2.28}$$

$$\frac{dW}{dt} = \widehat{L}_\mu W + M_\mu(W)\tag{2.29}$$

where $\widehat{L}_\mu W = L_\mu W - \zeta_1^*(W)\zeta_0$. The operator \widehat{L}_{μ_0} acting on \mathbb{H}_1 has the same spectrum as L_{μ_0} except that 0 is now a triple eigenvalue instead of a quadruple eigenvalue. One

can check that

$$\widehat{L}_{\mu_0}\zeta_1 = 0, \quad \widehat{L}_{\mu_0}\zeta_2 = \zeta_1, \quad \widehat{L}_{\mu_0}\zeta_3 = \zeta_2, \quad \zeta_3^*(\widehat{L}_{\mu_0}W) = 0. \quad (2.30)$$

Hence we have a three-dimensional center manifold on which solutions are given by

$$W = A\zeta_1 + B\zeta_2 + C\zeta_3 + \Phi_\mu(A, B, C). \quad (2.31)$$

Here Φ_μ takes values in \mathbb{D}_1 . Note that this implies solutions on the center manifold correspond with solutions of eq. (2.4), as desired. We also have that Φ_μ (1) has the same regularity as V' , (2) satisfies $\zeta_k^*(\Phi_\mu) = 0$ for $k = 1, 2, 3$, and (3) is at least quadratic in its arguments.

It is at this point that our discussion diverges from the work in (Iooss, 2000). From this point, Iooss uses the reversibility of the vector field and results from normal form theory to study the existence of homoclinic, heteroclinic, and periodic solutions on the center manifold. However, since there is an unspecified change of coordinates, the results in (Iooss, 2000) do not give quantitative estimates but rather qualitative descriptions of the solutions. For our purposes though, we would like to compare the profile of the travelling wave solutions and compare it to the mKdV kink solution, and so we must proceed differently. We shall instead compute the Taylor expansion of Φ_μ up to a certain order and get an explicit representation of the center manifold (up to some specified error).

We assume that Φ_μ can be written as a Taylor series in A, B, C , and μ :

$$\Phi_\mu(A, B, C) = \sum_{i,j,k,\ell} (\mu - 1)^\ell A^i B^j C^k \Phi_{ijk}^{(\ell)} \quad (2.32)$$

Note that the μ terms are centered at $\mu_0 = 1$. We will only need to compute up to some of the cubic terms, so we do not need Φ_μ is analytic as suggested by eq. (2.32). In fact $\Phi_\mu \in C^4$ in a neighborhood of $(\mu, A, B, C) = (1, 0, 0, 0)$ is sufficient and is

guaranteed by the regularity we assumed for V' and g .

It is useful to compute \widehat{L}_μ applied to each eigenvector:

$$\widehat{L}_\mu \zeta_1 = 0 \quad (2.33)$$

$$\widehat{L}_\mu \zeta_2 = \zeta_1 + (\mu - 1) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad (2.34)$$

$$\widehat{L}_\mu \zeta_3 = \zeta_2. \quad (2.35)$$

Note that these calculations agree with eq. (2.30) when μ is equal to $\mu_0 = 1$. Now plugging eq. (2.31) into eq. (2.29) gives

$$\begin{aligned} \dot{A}\zeta_1 + \dot{B}\zeta_2 + \dot{C}\zeta_3 + D\Phi_\mu(A, B, C) \begin{bmatrix} \dot{A} \\ \dot{B} \\ \dot{C} \end{bmatrix} = \\ B\zeta_1 + B(\mu - 1) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + C\zeta_3 + L_{\mu_0}\Phi_\mu(A, B, C) \\ + (2(1 - \mu)\Phi_\mu^x + (\mu - 1)(\delta^1\Phi_\mu^X + \delta^{-1}\Phi_\mu^X)) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \\ + \mu \left(g(A + \frac{1}{2}B + \frac{1}{6}C + (\delta^1\Phi_\mu^X - \Phi_\mu^x)) - g(A - \frac{1}{2}B + \frac{1}{6}C + (\Phi_\mu^x - \delta^{-1}\Phi_\mu^X)) \right) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \end{aligned} \quad (2.36)$$

where we represent the components of Φ_μ by $(\Phi_\mu^x, \Phi_\mu^\xi, \Phi_\mu^X)^T$. Now we can group the ζ_1 , ζ_2 and ζ_3 together – as well as the remaining terms – to get a system of differential

equations on the center manifold:

$$\dot{A} = B + \frac{2}{5} [\dots] \quad (2.37)$$

$$\dot{B} = C \quad (2.38)$$

$$\dot{C} = -12 [\dots] \quad (2.39)$$

$$D\Phi_\mu(A, B, C) \begin{bmatrix} \dot{A} \\ \dot{B} \\ \dot{C} \end{bmatrix} = L_{\mu_0} \Phi_\mu + [\dots] \begin{bmatrix} 0 \\ \frac{3}{5} \\ 2v^3 - \frac{2}{5}v \end{bmatrix}. \quad (2.40)$$

The \dots within the brackets are given the following expression

$$\begin{aligned} & B(\mu - 1) + 2(1 - \mu)\Phi_\mu^x + (\mu - 1)(\delta^1\Phi_\mu^X + \delta^{-1}\Phi_\mu^X) \\ & + \mu \left(g\left(A + \frac{1}{2}B + \frac{1}{6}C + (\delta^1\Phi_\mu^X - \Phi_\mu^x)\right) - g\left(A - \frac{1}{2}B + \frac{1}{6}C + (\Phi_\mu^x - \delta^{-1}\Phi_\mu^X)\right) \right), \end{aligned} \quad (2.41)$$

which we abridged to improve legibility. Now using the expression for the derivatives in eqs. (2.37) to (2.39) and plugging into eq. (2.40) gives the following:

$$\frac{\partial\Phi}{\partial A} \left(B + \frac{2}{5} [\dots] \right) + \frac{\partial\Phi}{\partial B} C + \frac{\partial\Phi}{\partial C} (-12 [\dots]) = L_{\mu_0} \Phi_\mu + [\dots] \begin{bmatrix} 0 \\ \frac{3}{5} \\ 2v^3 - \frac{2}{5}v \end{bmatrix}. \quad (2.42)$$

We will now assume Φ_μ has the form given in eq. (2.32). From the center manifold theorem, we have that the first-order terms and the terms quadratic in just A , B , and C are zero. Thus we start by first computing the second-order terms where $\ell = 1$. We get the following set of equations:

$$\Phi_{100}^{(1)} = L_{\mu_0} \Phi_{010}^{(1)} + \begin{bmatrix} 0 \\ \frac{3}{5} \\ 2v^3 - \frac{2}{5}v \end{bmatrix} \quad (2.43)$$

$$\Phi_{010}^{(1)} = L_{\mu_0} \Phi_{001}^{(1)} \quad (2.44)$$

$$0 = L_{\mu_0} \Phi_{100}^{(1)} \quad (2.45)$$

Equation (2.45) can be solved by noting that ζ_0 is the only zero eigenfunction for L_{μ_0} and $\zeta_0^*(\Phi_{100}^{(1)}) = 0$ since Φ_μ takes values in \mathbb{D}_1 , thus $\Phi_{100}^{(1)} = 0$. Then eq. (2.43) is reduced to

$$0 = L_{\mu_0} \Phi_{010}^{(1)} + \begin{bmatrix} 0 \\ \frac{3}{5} \\ 2v^3 - \frac{2}{5}v \end{bmatrix}, \quad (2.46)$$

which can be solved by integrating to get

$$\Phi_{010}^{(1)} = \begin{bmatrix} 0 \\ 0 \\ -\frac{1}{2}v^4 + \frac{1}{5}v^2 \end{bmatrix} + k\zeta_0 \quad (2.47)$$

for some $k \in \mathbb{R}$. Imposing the constraint that $\zeta_0^*(\Phi_{010}^{(1)}) = 0$ gives us that

$$k = -13/2100.$$

Similarly integrating eq. (2.44) gives

$$\Phi_{001}^{(1)} = \begin{bmatrix} 0 \\ 0 \\ -\frac{1}{10}v^5 + \frac{1}{15}v^3 \end{bmatrix} + k\zeta_1 \quad (2.48)$$

with the same value of k .

One can similarly compute the cubic coefficient $\Phi_{300}^{(0)}$ and get that

$$\Phi_{300}^{(0)} = 0. \quad (2.49)$$

We will not need to compute any of the other coefficients. As we will soon see, after a change of variables they end up being in the higher order terms to be neglected. Before proceeding, we will need a new parameterization for the center manifold. We let $\epsilon > 0$ correspond with the amplitude of our travelling wave solution, and look to write $\mu = c^{-2}$ in terms of ϵ . As seen in (Iooss, 2000), the heteroclinic orbits on the center manifold will only exists for c^2 slightly less than 1. Based on some formal calculations, it appears $c^2 = 1 - \epsilon^2/12$ will be the correct scaling. This will be borne

out by the coming calculations. Thus we have

$$\mu - 1 = c^{-2} - 1 = \frac{1}{1 - \epsilon^2/12} - 1 = \frac{\epsilon^2}{12} + \mathcal{O}(\epsilon^4).$$

Since we are looking for ϵ -amplitude waves with wavelength of order ϵ^{-1} , we make the following change of variables:

$$A(t) = \epsilon \underline{A}(\epsilon t), \quad B(t) = \epsilon^2 \underline{B}(\epsilon t), \quad \epsilon^3 \underline{C}(\epsilon t). \quad (2.50)$$

Then the equations of motion on the center manifold become

$$\begin{aligned} \underline{A}' &= \underline{B} + \mathcal{O}(\epsilon) \\ \underline{B}' &= \underline{C} \\ \underline{C}' &= -\underline{B} + 6\underline{A}^2 \underline{B} + \mathcal{O}(\epsilon). \end{aligned} \quad (2.51)$$

Here the $\mathcal{O}(\epsilon)$ represents functions that are at least C^4 in ϵ , \underline{A} , \underline{B} , and \underline{C} and can be bounded by a constant times ϵ when we are on bounded domains and $\epsilon > 0$ sufficiently small. Since we will be looking for bounded solutions on the center manifold, these terms can be controlled. We may upgrade this to $\mathcal{O}(\epsilon^2)$ if we additionally have $V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4 + \mathcal{O}(x^6)$ as $x \rightarrow 0$.

We shall consider three different assumptions on the potential going forward:

$$(H1) \quad V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4 + \mathcal{O}(\epsilon^5)$$

$$(H2) \quad V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4 + \mathcal{O}(\epsilon^6)$$

$$(H3) \quad V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4$$

The arguments for each assumption are similar, but stronger assumptions on the potential gives better estimates on the final result.

For (H1), we have that the flow on the center manifold is given by

$$\begin{aligned}
\underline{A}' &= \underline{B} + \epsilon F_1(\underline{A}, \underline{B}, \underline{C}; \epsilon) \\
\underline{B}' &= \underline{C} \\
\underline{C}' &= -\underline{B} + 6\underline{A}^2 \underline{B} + \epsilon G_1(\underline{A}, \underline{B}, \underline{C}; \epsilon) \\
\epsilon' &= 0
\end{aligned} \tag{2.52}$$

where F_1 and G_1 will be C^4 for $\epsilon > 0$ and $\mathcal{O}(1)$ as $\epsilon \rightarrow 0$. The additional equation $\epsilon' = 0$ is added so that we may use ϵ as an additional coordinate in our results. Note that this will not change the flow on the center manifold since ϵ remains fixed. For (H2) and (H3), we parameterize based on $\eta = \epsilon^2$ and the flow is now given by

$$\begin{aligned}
\underline{A}' &= \underline{B} + \eta F_2(\underline{A}, \underline{B}, \underline{C}; \sqrt{\eta}) \\
\underline{B}' &= \underline{C} \\
\underline{C}' &= -\underline{B} + 6\underline{A}^2 \underline{B} + \eta G_2(\underline{A}, \underline{B}, \underline{C}; \sqrt{\eta}) \\
\eta' &= 0
\end{aligned} \tag{2.53}$$

where F_2 and G_2 will be C^4 for $\eta > 0$ and $\mathcal{O}(1)$ as $\eta \rightarrow 0$. Reparameterizing to η will ultimately allow us to improve our error from $\mathcal{O}(\epsilon)$ to $\mathcal{O}(\epsilon^2)$. The systems can be extended to C^1 flows for negative values of the parameters: for instance we make the replacement

$$\begin{aligned}
\epsilon F_1(\underline{A}, \underline{B}, \underline{C}; \epsilon) &\rightarrow \epsilon F_1(\underline{A}, \underline{B}, \underline{C}; |\epsilon|) \\
\epsilon G_1(\underline{A}, \underline{B}, \underline{C}; \epsilon) &\rightarrow \epsilon G_1(\underline{A}, \underline{B}, \underline{C}; |\epsilon|)
\end{aligned} \tag{2.54}$$

to get eq. (2.52) is C^1 for (possibly negative) ϵ near zero. A similar replacement of $\sqrt{\eta} \rightarrow \sqrt{|\eta|}$ makes eq. (2.53) C^1 for η near zero.

The arguments for the persistence of heteroclinic orbits is similar for eqs. (2.52) and (2.53), so we will focus first on the former system and note where the results differ for the latter system.

2.3 Existence of Heteroclinic Orbit

At this point, our goal is to show the existence of a heteroclinic orbit for eq. (2.51) for $\epsilon > 0$ sufficiently small and to get estimates of the solution. One might expect that the flow on the center manifold for $\epsilon > 0$ small is well approximated by formally setting $\epsilon = 0$. Indeed, if we let $\epsilon = 0$, then the ODEs in eq. (2.51) become equivalent to the third-order differential equation

$$\underline{A}''' + \underline{A}' - 6\underline{A}^2 \underline{A}' = 0 \quad (2.55)$$

which has the solution

$$\underline{A}(s) = \frac{1}{\sqrt{2}} \tanh\left(\frac{s}{\sqrt{2}}\right). \quad (2.56)$$

This solution is the profile for the kink solution of the defocusing mKdV, ϕ . This represents a heteroclinic orbit for the system of ODEs since $(\underline{A}(s), \underline{B}(s), \underline{C}(s)) \rightarrow (\pm 1/\sqrt{2}, 0, 0)$ as $s \rightarrow \pm\infty$. One might expect that for $\epsilon > 0$ that there is also a heteroclinic orbit that is close to the above solution. Thus we want to show that the heteroclinic orbit at $\epsilon = 0$ persists for small perturbations of ϵ , and we want to get estimates of these orbits relative to ϵ . To get these results, we apply Fenichel theory. Review section 1.1 for the relevant results that will be used.

The idea behind the proof is to show that there is an overflowing invariant set with an unstable manifold and a corresponding inflowing invariant set with a stable manifold. We then show that at $\epsilon = 0$ these manifolds intersect transversally at a point, and that this intersection is given by the above heteroclinic orbit. From there, we show that this intersection is preserved for $\epsilon > 0$ and the heteroclinic orbit remains $\mathcal{O}(\epsilon)$ or $\mathcal{O}(\epsilon^2)$ to the original orbit.

2.3.1 The Unstable and Stable Manifolds

We first must find the appropriate overflowing invariant set.¹ From the heteroclinic orbit found for $\epsilon = 0$, we know that $(\underline{A}, \underline{B}, \underline{C}, \epsilon) = (-1/\sqrt{2}, 0, 0, 0)$ should be one point in the set. In fact, for fixed $\epsilon > 0$ we have that multiples of ζ_1 are fixed points for eq. (2.29). From the center manifold theorem in (Vanderbauwhede and Iooss, 1992), bounded solutions sufficiently close to the origin will lie exactly on the center manifold. Thus for $\epsilon > 0$ sufficiently close to zero, any closed interval on the \underline{A} -axis is composed entirely of fixed points on the center manifold. We will choose $\epsilon_0 > 0$ small enough such that for $\epsilon \in (0, \epsilon_0]$ the \underline{A} -axis from $[-1, 1]$ is composed entirely of fixed points.

If we fix a small $\delta > 0$ and set $A_{-\infty} = -1/\sqrt{2}$, then

$$\overline{M} = \{(\underline{A}, 0, 0, \epsilon) \in \mathbb{R}^4 : |(\underline{A} - A_{-\infty}, \epsilon)| \leq \delta\} \quad (2.57)$$

is a smooth manifold with boundary that is invariant under the flow in eq. (2.52). In fact, \overline{M} consists exclusively of fixed points of the flow.

To get apply theorem 1 and get an unstable manifold for \overline{M} we need that

- (i) \overline{M} is overflowing invariant, and
- (ii) the generalized Lyapunov-type numbers on \overline{M} satisfy the inequalities in theorem 1.

As written, \overline{M} is *not* an overflowing invariant manifold. However, a common trick in Fenichel is to adjust the flow on the boundary of an invariant manifold so that it becomes overflowing invariant (see (Wiggins, 1994, §6.3)). This will alter the behavior of our dynamical system at the boundary, but elsewhere the dynamics will remain

¹We need also to find the inflowing invariant set, but we can rely on the symmetry of eq. (2.51) to get this. In fact, we will regularly rely on the symmetry of the flow to get many of the results for the inflowing invariant set after working it out for the overflowing invariant set.

the same. For our case, we may adjust the flow near the boundary $|(\underline{A} - A_{-\infty}, \epsilon)| = \delta$ to get \overline{M} is overflowing invariant, but this will not affect the dynamics near the heteroclinic orbit. Thus we can still talk about the existence of the heteroclinic orbit in the unaltered system. This adjustment will need to be done in a way to not greatly affect the generalized Lyapunov-type numbers. For now, we set aside point (i) and address (ii), which is more straightforward.

Since \overline{M} consists only of fixed points, the generalized Lyapunov-type numbers can be computed using the linearization of the flow. Note that since each $(\underline{A}, 0, 0, \epsilon) \in \overline{M}$ is a fixed point, we have that

$$\begin{aligned} F_1(\underline{A}, 0, 0, \epsilon) &= 0 \\ G_1(\underline{A}, 0, 0, \epsilon) &= 0 \end{aligned} \tag{2.58}$$

and the partial derivatives of F_1 and G_1 with respect to \underline{A} or ϵ will be zero. Thus at a point $(\underline{A}, 0, 0, \epsilon) \in \overline{M}$, the linearization of the flow is given by

$$\begin{bmatrix} 0 & 1 + \epsilon \frac{\partial F_1}{\partial \underline{B}}(\underline{A}, 0, 0; \epsilon) & \epsilon \frac{\partial F_1}{\partial \underline{C}}(\underline{A}, 0, 0; \epsilon) & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 6\underline{A}^2 - 1 + \epsilon \frac{\partial G_1}{\partial \underline{B}}(\underline{A}, 0, 0; \epsilon) & \epsilon \frac{\partial G_1}{\partial \underline{C}}(\underline{A}, 0, 0; \epsilon) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{2.59}$$

The tangent space at $p \in M$ is given by $T_p M = \text{span}\{(1, 0, 0, 0), (0, 0, 0, 1)\}$. The vector bundles N^u and N^s will be defined as the unstable and stable subspaces of each fixed point, respectively. That these vector bundles are invariant under the flow and continuous follows immediately from their definition. The two eigenvalues $\lambda_1, \lambda_2 = 0$ correspond with the flow tangent to the manifold. Fixing $\underline{A} = A_{-\infty}$ and $\epsilon = 0$, the other eigenvalues are $\lambda_{3,4} = \pm \sqrt{6A_{-\infty}^2 - 1}$, which correspond with the flow along the vector bundles N^u and N^s , respectively. There at $p_0 = (A_{-\infty}, 0, 0, 0)$ we have the generalized Lyapunov-type numbers given by

$$\lambda^u(p_0) = \nu^s(p_0) = \exp\left(-\sqrt{6A_{-\infty}^2 - 1}\right), \quad \sigma^s(p_0) = 0. \tag{2.60}$$

To have a C^1 unstable manifold, we are required to have $\lambda^u(p), \nu^s(p), \sigma^s(p) < 1$ for each point $p \in M$. By the continuity of eigenvalues, we can guarantee this by choosing δ small enough.

Then condition (ii) is satisfied. Now we want to show that we can alter near ∂M so that (i) is also satisfied without causing (ii) to become invalid. We first introduce a C^∞ bump function, $\chi : [0, \infty) \rightarrow \mathbb{R}$, such that

- (1) $0 \leq \chi(r) \leq 1$ for $r \in [0, \infty)$
- (2) $\chi(r) = 0$ when $r \in [0, \delta - \sigma]$
- (3) $\chi(r) = 1$ when $r \in [\delta - \frac{\sigma}{2}, \delta + \frac{\sigma}{2}]$
- (4) $\chi(r) = 0$ when $r \in [\delta + \sigma, \infty)$

where $\sigma > 0$ will be a parameter that we can make as small as necessary. We then alter the vector field in eq. (2.52) by setting

$$\begin{aligned}
 \underline{A}' &= \underline{B} + \epsilon F_1(\underline{A}, \underline{B}, \underline{C}; \epsilon) + \chi(|(\underline{A} - A_{-\infty}, \epsilon)|) \cdot (\underline{A} - A_{-\infty}) \\
 \underline{B}' &= \underline{C} \\
 \underline{C}' &= -\underline{B} + 6\underline{A}^2 \underline{B} + \epsilon G_1(\underline{A}, \underline{B}, \underline{C}; \epsilon) \\
 \epsilon' &= \chi(|(\underline{A} - A_{-\infty}, \epsilon)|) \cdot \epsilon.
 \end{aligned} \tag{2.61}$$

This change keeps the flow C^1 and makes \overline{M} an overflowing invariant vector field. However, a couple things need to be checked before applying theorem 1: the vector bundles N^u and N^s must be defined on $\chi \neq 0$ and the generalized Lyapunov-type numbers must satisfy the necessary inequalities.

The extension of the normal vector bundles is somewhat technical, but otherwise straightforward. We need N^u and N^s invariant under the flow and continuous. In particular, if p is a point in M where $\chi \neq 0$ and $\xi \in N_p^u$, then $D\phi_t(p)\xi \in N_{\phi_t(p)}^u$ for

all t such that $\phi_t(p) \in M$. A similar result should hold for N^s . We also need that the vector bundles are continuous with respect to p . Continuity relies on showing that we can assign the vector bundles in a way so that if $\phi_t(p) \rightarrow p'$ as $t \rightarrow -\infty$ then $N_{\phi_t(p)}^u$ approaches $N_{p'}^u$. This can be done and the details are carried out in appendix A.

For the generalized Lyapunov-type numbers, it can be shown that the values on the altered region of M can be bounded by those on the unaltered region. More generally, we have the following result.

Proposition 1. *Let $K \subset M$ be a compact set. If $p \in M$ such that $\phi_{-t}(p) \rightarrow K$ as $t \rightarrow \infty$, then*

- (i) $\lambda^u(p) \leq \lambda^u(K)$,
- (ii) $\nu^s(p) \leq \nu^s(K)$, and
- (iii) if $\nu^s(K) < 1$, then $\sigma^s(p) \leq \sigma^s(K)$.

The proof is give in appendix A and follows similarly to the arguments found in (Dieci and Lorenz, 1997).

We can therefore conclude that $W_{\text{loc}}^u(\overline{M})$ exists. If we set $A_\infty = 1/\sqrt{2}$, then an analogous argument holds for showing that

$$\overline{N} = \{(\underline{A}, 0, 0, \epsilon) \in \mathbb{R}^4 : |(\underline{A} - A_\infty, \epsilon)| \leq \delta\} \quad (2.62)$$

has a *stable* manifold, $W_{\text{loc}}^s(\overline{N})$.

2.3.2 Transversal intersection at $\epsilon = 0$

To show a heteroclinic orbit exists for $\epsilon > 0$, we first show that stable and unstable manifolds described above have a transverse intersection at $\epsilon = 0$. This intersection then persists for perturbations in ϵ (since the manifolds are C^1 with respect to ϵ) and thus implies the existence of the heteroclinic orbit.

The heteroclinic orbit at $\epsilon = 0$ can be found explicitly. The dynamics (away from where we modified the vector field) are given by

$$\begin{aligned}\underline{A}' &= \underline{B} \\ \underline{B}' &= \underline{C} \\ \underline{C}' &= -\underline{B} + 6\underline{A}^2\underline{B}.\end{aligned}\tag{2.63}$$

The system of ODEs in eq. (2.63) has two invariants:

$$I_1(\underline{A}, \underline{B}, \underline{C}) = \underline{C} + \underline{A} - 2\underline{A}^3 \tag{2.64}$$

$$I_2(\underline{A}, \underline{B}, \underline{C}) = \frac{1}{2}\underline{B}^2 + \frac{1}{2}\underline{A}^2 - \frac{1}{2}\underline{A}^4 - \underline{A}I_1(\underline{A}, \underline{B}, \underline{C}). \tag{2.65}$$

We then look for solutions on the manifolds given by

$$I_1(A_{-\infty}, 0, 0) = 0 \quad \text{and} \quad I_2(A_{-\infty}, 0, 0) = \frac{1}{8}. \tag{2.66}$$

The above equations and the fact that $\underline{B} = \underline{A}'$ gives us that \underline{A} must satisfy the following first order ODE:

$$(\underline{A}')^2 = \left(\frac{1}{2} - \underline{A}^2\right)^2, \tag{2.67}$$

which can be solved by separation of variables. The solutions are thus

$$\underline{A}(s) = \pm \frac{1}{\sqrt{2}} \tanh\left(\frac{s}{\sqrt{2}}\right) \tag{2.68}$$

up to a shift in the variable s . One can check that these are solutions of eq. (2.63) (taking $\underline{B} = \underline{A}'$ and $\underline{C} = \underline{A}''$) and define two heteroclinic orbits: one traveling from $A_{-\infty}$ to A_{∞} and one traveling from A_{∞} to $A_{-\infty}$. Let

$$\gamma_{\pm}(t) = \begin{bmatrix} \pm \frac{1}{\sqrt{2}} \tanh\left(\frac{s}{\sqrt{2}}\right) \\ \pm \frac{1}{2} \text{sech}^2\left(\frac{s}{\sqrt{2}}\right) \\ \mp \frac{1}{\sqrt{2}} \tanh\left(\frac{s}{\sqrt{2}}\right) \text{sech}^2\left(\frac{s}{\sqrt{2}}\right) \end{bmatrix} = \begin{bmatrix} \pm \phi(s) \\ \pm \phi'(s) \\ \pm \phi''(s) \end{bmatrix} \tag{2.69}$$

denote the two heteroclinic orbits.

The solution corresponding with the choice of $+$ also lies inside the manifolds $W_{\text{loc}}^u(\overline{M})$ and $W_{\text{loc}}^s(\overline{N})$ since it converges to \overline{M} and \overline{N} as $s \rightarrow -\infty$ and $s \rightarrow +\infty$, respectively. This does not imply the local manifolds intersect since they are only defined in a neighborhood of \overline{M} and \overline{N} , but we may extend these manifolds under the flow so that they both contain the point $(\epsilon, \underline{A}, \underline{B}, \underline{C}) = (0, 0, 1/2, 0)$ and thus intersect. We shall refer to the manifolds extended under the flow by \mathcal{M}_ϵ and \mathcal{N}_ϵ . These extended manifolds are still C^1 with respect to the parameter ϵ .

Now the goal is to demonstrate that this intersection is transverse. That is for $p = (0, 1/2, 0)$ we want to show that $T_p\mathcal{M}_0 + T_p\mathcal{N}_0 = T_p\mathbb{R}^3$. One can explicitly compute each of the tangent spaces at p and show they span $T_p\mathbb{R}^3$. This is done by finding the intersection each of these manifolds make with the \underline{BC} -plane. Similar to the construction of the heteroclinic orbit, we find the orbit which approaches some asymptotic value on the \underline{A} -axis near $A_{-\infty}$ or A_∞ and find where it intersect the \underline{BC} -plane. These orbits lie on the stable and unstable manifolds, and so this shows how the manifolds intersect the plane.

Take ω to be a point near $A_{-\infty} = -1/\sqrt{2}$. The orbit that approaches $(\omega, 0, 0)$ in backwards time lies on the intersection of

$$\begin{aligned} I_1(\underline{A}, \underline{B}, \underline{C}) &= I_1(\omega, 0, 0) = \omega - 2\omega^3 \\ I_2(\underline{A}, \underline{B}, \underline{C}) &= I_2(\omega, 0, 0) = -\frac{1}{2}\omega^2 + \frac{3}{2}\omega^4. \end{aligned} \tag{2.70}$$

Setting $\underline{A} = 0$, we can find that \mathcal{M}_0 hits the \underline{BC} - plane at

$$\mu(\omega) = (0, |\omega|\sqrt{3\omega^2 - 1}, \omega - 2\omega^3) \tag{2.71}$$

for ω close to $A_{-\infty}$. In particular, we see that if $\mu(A_{-\infty}) = p$. Identical reasoning

gives that \mathcal{N}_0 intersects the plane at

$$\nu(\alpha) = (0, |\alpha|\sqrt{3\alpha^2 - 1}, \alpha - 2\alpha^3) \quad (2.72)$$

where α is near $A_\infty = 1/\sqrt{2}$ and $\nu(A_\infty) = p$.

The derivative of the heteroclinic orbit is given by $(1/2, 0, -1/2)$, and this vector lies in both $T_p\mathcal{M}_0$ and $T_p\mathcal{N}_0$. Since $\mu(\omega) \in \mathcal{M}_0$ for ω near A_∞ , we have that

$$\mu'(A_\infty) = \left(0, 1, \frac{1}{\sqrt{2}}\right) \in T_p\mathcal{M}_0. \quad (2.73)$$

Similarly,

$$\nu'(A_\infty) = \left(0, 1, \frac{-1}{\sqrt{2}}\right) \in T_p\mathcal{N}_0. \quad (2.74)$$

Therefore

$$T_p\mathcal{M}_0 + T_p\mathcal{N}_0 = \text{span} \left\{ \left(\frac{1}{2}, 0, \frac{-1}{2}\right), \left(0, 1, \frac{1}{\sqrt{2}}\right), \left(0, 1, \frac{-1}{\sqrt{2}}\right) \right\} = T_p\mathbb{R}^3 \quad (2.75)$$

and the intersection is transverse. This implies that there is a heteroclinic orbit on the intersection of \mathcal{M}_ϵ and \mathcal{N}_ϵ for $\epsilon > 0$.

2.3.3 Estimates on the heteroclinic orbit

From the previous section, we have the existence of heteroclinic orbits that are perturbation of γ_\pm at $\epsilon = 0$. From the C^1 regularity of the manifolds with respect to the coordinates, we expect that the orbits remain $\mathcal{O}(\epsilon)$ close to the unperturbed orbits in some sense. There are some subtleties to be addressed. The manifolds remain $\mathcal{O}(\epsilon)$ close in Hausdorff distance, but this does not imply the orbits on the manifolds remain $\mathcal{O}(\epsilon)$ close for all time. The dynamics on the manifolds might change causing orbits on the perturbed manifold to diverge asymptotically despite remaining close initially.

First, let us introduce notation for the perturbed heteroclinic orbits. We shall

denote by $\gamma_{\pm,\epsilon} = (A_{\pm,\epsilon}, B_{\pm,\epsilon}, C_{\pm,\epsilon})$ to be the perturbations of γ_{\pm} for $\epsilon > 0$, where we set $\gamma_{\pm,\epsilon}(0)$ to be the point where the orbits cross the \underline{BC} -plane. From the continuity of the manifolds with respect to ϵ , we have that $|\gamma_{\pm,\epsilon}(0) - \gamma_{\pm}(0)| = \mathcal{O}(\epsilon)$ for small ϵ . We can extend this estimate onto arbitrarily large time scales by applying an argument using the Gröwall inequality. That is, for every $T > 0$ we have for sufficiently small ϵ that $|\gamma_{\pm,\epsilon}(s) - \gamma_{\pm}(s)| = C\epsilon$ for all $s \in [-T, T]$, where $C > 0$ is independent of s .

This argument is insufficient for extending the estimate to all time. To get that the orbits remain close as $s \rightarrow \pm\infty$, we can rely on part 7 of theorem 2. Taking (ϵ, ω) sufficiently close to $(0, A_{-\infty})$ as base points, the theorem states that the unstable manifold is C^1 with respect to (ϵ, ω) . Note that the overflowing invariant manifold (away from the bump function) consists only of fixed points, so orbits on the unstable manifold approach a unique fixed point given by (ϵ, ω) . Take $T > 0$ large enough so that all the points on \mathcal{M}_{ϵ} (for $\epsilon \leq \epsilon_0$) which intersect the \underline{BC} -plane are in the local unstable manifold when flowed backward in time by $-T$ units. Then locally, there is a one-to-one correspondence between these points flowed backward in time and the points in \overline{M} ; furthermore, this correspondence is C^1 due to theorem 2. This implies that if the points flowed backward are $\mathcal{O}(\epsilon)$ close then there backward limits are $\mathcal{O}(\epsilon)$ close as well. In particular, the backward limits of $\gamma_{+,\epsilon}$ and γ_+ are $\mathcal{O}(\epsilon)$ close. The argument for the stable manifold is analogous. This shows that the heteroclinic orbits remain $\mathcal{O}(\epsilon)$ for all time. In the case where $V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4 + \mathcal{O}(\epsilon^6)$, this can be upgraded to $\mathcal{O}(\epsilon^2)$; the proof is similar but we use the regularity of the manifolds with respect to $\eta = \epsilon^2$ instead. Therefore, we have the following.

Proposition 2. *There exists $\epsilon_0 > 0$ such that for every $\epsilon \in (0, \epsilon_0]$ there exist two heteroclinic orbits $\gamma_{\pm,\epsilon}$ of eq. (2.52) such that*

$$|\gamma_{\pm,\epsilon}(s) - \gamma_{\pm}(s)| \leq C\epsilon \quad \text{for all } s \in \mathbb{R} \quad (2.76)$$

where γ_{\pm} are defined in eq. (2.69). If $V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4 + \mathcal{O}(\epsilon^6)$, then we instead

have the estimate

$$|\gamma_{\pm,\epsilon}(s) - \gamma_{\pm}(s)| \leq C\epsilon^2 \quad \text{for all } s \in \mathbb{R}. \quad (2.77)$$

By starting to unravel the change of coordinates, we can show the existence of solutions to the advance-delay equation of the form

$$x_{\pm,\epsilon}(t) = q_{\pm,\epsilon}(t) + (\Phi_{\mu}(\epsilon A_{\pm,\epsilon}(\epsilon t), \epsilon^2 B_{\pm,\epsilon}(\epsilon t), \epsilon^3 C_{\pm,\epsilon}(\epsilon t)))_x \quad (2.78)$$

where $q_{\pm,\epsilon}(t)$ satisfies the differential equation

$$\frac{dq_{\pm,\epsilon}}{dt} = \epsilon A_{\pm,\epsilon}(\epsilon t). \quad (2.79)$$

The differential equation for q comes from eq. (2.28) and the fact that $\zeta_1^*(\Phi_{\mu}) = 0$.

Taking a derivative we also have

$$\dot{x}_{\pm,\epsilon}(t) = \epsilon A_{\pm,\epsilon}(\epsilon t) + (\Phi_{\mu}(\epsilon A_{\pm,\epsilon}(\epsilon t), \epsilon^2 B_{\pm,\epsilon}(\epsilon t), \epsilon^3 C_{\pm,\epsilon}(\epsilon t)))_{\xi}. \quad (2.80)$$

The coordinates $A_{\pm,\epsilon}$, $B_{\pm,\epsilon}$, and $C_{\pm,\epsilon}$ are at least C^5 and Φ_{μ} is at least C^4 .

The main result will be stated by writing eq. (2.2) in terms of the strain variables, $u_n = x_{n+1} - x_n$. That is, we look at the travelling wave solution given by

$$x_{\pm,\epsilon}(n+1 - c\tilde{t}) - x_{\pm,\epsilon}(n - c\tilde{t}). \quad (2.81)$$

Using a central finite difference, we get that

$$\begin{aligned} x_{\pm,\epsilon}(t+1) - x_{\pm,\epsilon}(t) &= \dot{x}_{\pm,\epsilon}(t+1/2) + \int_{t+1/2}^{t+1} \ddot{x}_{\pm,\epsilon}(s)(t+1-s)^2 ds \\ &= \pm \epsilon \phi(\epsilon(t+1/2)) + \epsilon^2 R_{\epsilon,\pm}(\epsilon(t+1/2)) \end{aligned} \quad (2.82)$$

where $R_{\epsilon,\pm} \in C_b^3$. Thus (after shifting the solution) we have that there is a travelling

wave like solutions of the FPUT of the form

$$u_n(t) = \pm \epsilon \phi_{\epsilon, \pm}(\epsilon(n - ct)) + \epsilon^2 R_{\epsilon, \pm}(\epsilon(n - ct)) \quad (2.83)$$

Additionally, if (H2) holds we improve the error estimate so that there are solutions of the form

$$u_n(t) = \pm \epsilon \phi(\epsilon(n - ct)) + \epsilon^3 R_{\epsilon, \pm}(\epsilon(n - ct)). \quad (2.84)$$

To match similar estimates made in (Friesecke and Pego, 1999), one would expect the remainder terms to also be in a Sobolev space like H^1 . This is in general not true. The travelling wave solution found above may not approach a different limit asymptotically than $\epsilon \phi$, in which case the remainder does not approach zero asymptotically in space. A necessary condition to get $R_{\epsilon, \pm} \in H^1$ would be for u_n to approach the same limits given as $\pm \epsilon \phi(\epsilon(n - ct))$ as $|n| \rightarrow \infty$.

A useful tool for showing this is the following invariant for eq. (2.4):

$$\dot{x}(t) - \mu \int_t^{t+1} V'(x(s) - x(s-1)) ds. \quad (2.85)$$

It is easy to check that the above is constant for solutions of the advance-delay differential equation. If $\dot{x}(t) \rightarrow r_\infty$ as $t \rightarrow \infty$, then eq. (2.85) is equal to

$$r_\infty - \mu V'(r_\infty) \quad (2.86)$$

If we also have that $\dot{x}(t) \rightarrow r_{-\infty}$ as $t \rightarrow -\infty$, then we have eq. (2.85) is also equal to

$$r_{-\infty} - \mu V'(r_{-\infty}) \quad (2.87)$$

and so the limits $r_{\pm\infty}$ satisfy the equation

$$r_\infty - \mu V'(r_\infty) = r_{-\infty} - \mu V'(r_{-\infty}). \quad (2.88)$$

For arbitrary V , we cannot show that the limits agree with the limits of $\pm\epsilon\phi$. However, if we assume (H3) holds, i.e. that $V(x) = \frac{1}{2}x^2 - \frac{1}{24}x^4$, then we do have the limits agree. This follows in part from the oddness of V' . That is, we have from V' odd that $\lim_{s \rightarrow \infty} A_{\pm,\epsilon}(s) = -\lim_{s \rightarrow -\infty} A_{\pm,\epsilon}(s)$ and so $r_\infty = -r_{-\infty}$. Therefore, we must have that

$$r_\infty - \mu V'(r_\infty) = 0. \quad (2.89)$$

Given that $V'(x) = x - \frac{1}{6}x^3$, we have that the only solutions to the above equation are $r_\infty = 0, \pm\epsilon/\sqrt{2}$. This implies that the limits of the travelling wave solutions agree with $\pm\epsilon\phi$. Specifically, we must have $A_{\pm,\epsilon}(s) \rightarrow \pm 1/\sqrt{2}$ as $s \rightarrow \infty$ and $A_{\pm,\epsilon}(s) \rightarrow \mp 1/\sqrt{2}$ as $s \rightarrow -\infty$.

Appendix A

Extension of normal vector bundles

The proofs for these lemmas should be similar to the proofs found in (Dieci and Lorenz, 1997).

Lemma 1. *Let $p \in M$ with $\nu^s(p) < 1$. For $c > \sigma^s(p)$, we have*

$$\|A_t(p)\| \|B_t(p)\|^c \rightarrow 0 \quad \text{as } t \rightarrow \infty. \quad (\text{A.1})$$

Conversely, if eq. (A.1) holds for some $c \in \mathbb{R}$, then $c \geq \sigma^s(p)$.

Lemma 2. *For $p \in M$ and $s, t \geq 0$, we have the following:*

- (i) $A_{s+t}(p) = A_t(\phi_{-s}(p))A_s(p)$
- (ii) $B_{s+t}(p) = B_s(p)B_t(\phi_{-s}(p))$
- (iii) $C_{s+t}(p) = C_t(\phi_{-s}(p))C_s(p)$.

Proposition 1. *Let $K \subset M$ be a compact set. If $p \in M$ such that $\phi_{-t}(p) \rightarrow K$ as $t \rightarrow \infty$, then*

- (i) $\lambda^u(p) \leq \lambda^u(K)$,
- (ii) $\nu^s(p) \leq \nu^s(K)$, and
- (iii) if $\nu^s(K) < 1$, then $\sigma^s(p) \leq \sigma^s(K)$.

Proof. (i) Let $a \in \mathbb{R}$ such that $\lambda^u(K) < a$. For each $q \in K$ there is a $\tau_q > 0$ and an open, precompact neighborhood of q , U_q , such that

$$\|C_{\tau_q}(q')\| < a^{\tau_q} \quad \text{for all } q' \in U_q.$$

Then $\{U_q\}_{q \in K}$ is an open cover of K , and so we can take a finite subcover $\{U_i\}_{i=1}^m$ with associated τ_q values denoted by τ_i for $i = 1, \dots, m$. Let $U = \bigcup_{i=1}^m U_i$ and assume

without loss of generality that $\tau_1 \leq \tau_2 \leq \dots \leq \tau_m$. Since $\lambda^u(p)$ is constant along trajectories and $\phi_{-t}(p) \rightarrow K$ as $t \rightarrow \infty$, we can assume that $\phi_{-t}(p) \in U$ for all $t \geq 0$.

We can now break up the orbit of $\phi_{-t}(p)$ into discrete times to keep track of which U_i the orbit lies in. We shall do this inductively. Set $t_0 = 0$. Then $\phi_{-t_0}(p) = p \in U_{i_0}$ for some index $i_0 \in \{1, 2, \dots, m\}$. Then we can define $t_1 = t_0 + \tau_{i_0}$ and again we have $\phi_{-t_1}(p) \in U_{i_1}$ for some index i_1 . We can continue this process. Suppose we have t_k and τ_{i_k} . Then

$$t_{k+1} = t_k + \tau_{i_k}, \quad \phi_{-t_{k+1}}(p) \in U_{i_{k+1}},$$

and so we have t_{k+1} and $\tau_{i_{k+1}}$ defined. Note that $t_{k+1} - t_k = \tau_{i_k} \leq \tau_m$, so the distance between times does not grow too large. Furthermore, we also have $t_{k+1} - t_k = \tau_{i_k} \geq \tau_1$ and so $t_k \rightarrow \infty$ as $k \rightarrow \infty$.

Now suppose $t > 0$ is fixed and arbitrary. There is some ℓ such that $t_\ell \leq t < t_{\ell+1}$. Then there is some $s < \tau_m$ such that

$$\begin{aligned} t &= t_\ell + s \\ &= \sum_{k=0}^{\ell-1} \tau_{i_k} + s. \end{aligned} \tag{A.2}$$

Using this decomposition of t along with lemma 2, we get that

$$\begin{aligned} C_t(p) &= C_{t_\ell+s}(p) \\ &= C_s(\phi_{-t_\ell}(p))C_{t_\ell}(p) \\ &= C_s(\phi_{-t_\ell}(p))C_{\tau_{i_{\ell-1}}}(\phi_{-t_{\ell-1}}(p))C_{\tau_{i_{\ell-2}}}(\phi_{-t_{\ell-2}}(p)) \cdots C_{\tau_{i_0}}(p). \end{aligned} \tag{A.3}$$

Thus we have

$$\begin{aligned} \|C_t(p)\| &\leq \|C_s(\phi_{-t_\ell}(p))\| a^{\tau_{i_{\ell-1}}} \cdot a^{\tau_{i_{\ell-2}}} \cdots a^{\tau_{i_0}} \\ &= \|C_s(\phi_{-t_\ell}(p))\| a^{t_\ell}. \end{aligned} \tag{A.4}$$

Defining a constant C_1 by

$$C_1 = \max\{a^{-s}\|C_s(q)\| : q \in \overline{U}, 0 \leq s \leq \tau_m\} \tag{A.5}$$

we can write

$$\|C_t(p)\| \leq C_1 a^s a^{t_\ell} = C_1 a^t. \tag{A.6}$$

Since this C_1 is independent of t , raising both sides to $1/t$ and taking the limit as

$t \rightarrow \infty$ gives us that

$$\limsup_{t \rightarrow \infty} \|C_t(p)\|^{1/t} \leq a, \quad (\text{A.7})$$

and so $\lambda^u(p) \leq a$ for each $a > \lambda^u(K)$. This proves $\lambda^u(p) \leq \lambda^u(K)$.

(ii) We follow a similar argument for $\nu^s(p)$. Let $a \in \mathbb{R}$ such that $\nu^s(K) < a$. We can find an open cover of K given by $\{U_i\}_{i=1}^m$ (with each U_i precompact) and positive numbers $\tau_1 \leq \tau_2 \leq \dots \leq \tau_m$ such that

$$\|B_{\tau_i}(q)\| < a^{\tau_i} \quad \text{for all } q \in U_i. \quad (\text{A.8})$$

The number $\nu^s(p)$ is constant on orbits, so assume that $\phi_{-t}(p) \in U := \cup_{i=1}^m U_i$ for all $t \geq 0$. We can similarly construct the t_k and τ_{i_k} inductively.

Let $t > 0$. Then there is an ℓ such that $t_\ell \leq t < t_{\ell+1}$, and we have $0 \leq s < \tau_m$ with

$$\begin{aligned} t &= t_\ell + s \\ &= \sum_{k=0}^{\ell-1} \tau_{i_k} + s. \end{aligned} \quad (\text{A.9})$$

Thus

$$B_t(p) = B_{\tau_{i_0}}(p) B_{\tau_{i_1}}(\phi_{-t_1}(p)) \cdots B_{\tau_{i_{\ell-1}}}(\phi_{-t_{\ell-1}}(p)) B_s(\phi_{-t_\ell}(p)). \quad (\text{A.10})$$

We can then get

$$\|B_t(p)\| \leq \|B_s(\phi_{-t_\ell}(p))\| a^{t-s}. \quad (\text{A.11})$$

Defining a constant C_2 by

$$C_2 = \max\{a^{-s} \|B_s(q)\| : q \in \overline{U}, 0 \leq s \leq \tau_m\} \quad (\text{A.12})$$

we can write

$$\|B_t(p)\| \leq C_2 a^s a^{t_\ell} = C_2 a^t. \quad (\text{A.13})$$

Taking limits gives us $\nu^s(p) \leq a$ and thus $\nu^s(p) \leq \nu^s(K)$.

(iii) Assume that $\nu^p(K) < 1$. Let $c > \sigma^s(K)$ be arbitrary. For each $q \in K$, there is a τ_q and a precompact, open neighborhood of q , U_q , such that

$$\|A_{\tau_q}(q')\| \|B_{\tau_q}(q')\|^c \leq \frac{1}{2}, \quad \text{for all } q' \in U_q. \quad (\text{A.14})$$

We again take a finite subcover $\{U_i\}_{i=1}^m$ with corresponding $\tau_1 \leq \tau_2 \leq \dots \leq \tau_m$. The number $\sigma^s(p)$ is constant on orbits so assume that $\phi_{-t}(p) \in U := \cup_{i=1}^m U_i$ for all $t \geq 0$. The t_k and τ_{i_k} values are constructed the same way as in (i).

For $t > 0$, we have $t_\ell \leq t < t_{\ell+1}$ and we can write t as

$$\begin{aligned} t &= t_\ell + s \\ &= \sum_{k=0}^{\ell-1} \tau_{i_k} + s \end{aligned} \tag{A.15}$$

with $0 \leq s < \tau_m$. By our product formulas,

$$A_t(p) = A_s(\phi_{-t_\ell}(p)) A_{\tau_{i_{\ell-1}}}(\phi_{-t_{\ell-1}}(p)) A_{\tau_{i_{\ell-2}}}(\phi_{-t_{\ell-2}}(p)) \cdots A_{\tau_{i_0}}(p) \tag{A.16}$$

and

$$B_t(p) = B_{\tau_{i_0}}(p) B_{\tau_{i_1}}(\phi_{-t_1}(p)) \cdots B_{\tau_{i_{\ell-1}}}(\phi_{-t_{\ell-1}}(p)) B_s(\phi_{-t_\ell}(p)). \tag{A.17}$$

Thus

$$\|A_t(p)\| \|B_t(p)\|^c \leq C_3 \left(\frac{1}{2}\right)^\ell \tag{A.18}$$

where

$$C_3 = \max\{\|A_s(q)\| \|B_s(q)\|^c : q \in \overline{U}, 0 \leq s \leq \tau_m\}. \tag{A.19}$$

As $t \rightarrow \infty$, we have $\ell \rightarrow \infty$. Therefore $\|A_t(p)\| \|B_t(p)\|^c \rightarrow 0$ as $t \rightarrow \infty$ and $\sigma^s(p) \leq c$. We can then conclude that $\sigma^s(p) \leq \sigma^s(K)$. \square

References

- Bambusi, D. and Ponno, A. (2006). On metastability in FPU. *Communications in mathematical physics*, 264(2):539–561.
- Dieci, L. and Lorenz, J. (1997). Lyapunov-type numbers and torus breakdown: Numerical aspects and a case study. *Numerical Algorithms*, 14(1):79–102.
- Dumas, E. and Pelinovsky, D. (2014). Justification of the log-KdV equation in granular chains: The case of precompression. *SIAM Journal on Mathematical Analysis*, 46(6):4075–4103.
- Friesecke, G. and Pego, R. L. (1999). Solitary waves on FPU lattices: I. qualitative properties, renormalization and continuum limit. *Nonlinearity*, 12(6):1601.
- Hong, Y., Kwak, C., and Yang, C. (2021). On the Korteweg–de Vries limit for the Fermi–Pasta–Ulam system. *Archive for Rational Mechanics and Analysis*, 240(2):1091–1145.
- Iooss, G. (2000). Travelling waves in the Fermi-Pasta-Ulam lattice. *Nonlinearity*, 13(3):849.
- Iooss, G. and Kirchgässner, K. (2000). Travelling waves in a chain of coupled nonlinear oscillators. *Communications in Mathematical Physics*, 211(2):439–464.
- Kato, T. (2013). *Perturbation theory for linear operators*, volume 132. Springer Science & Business Media.
- Khan, A. and Pelinovsky, D. E. (2017). Long-time stability of small FPU solitary waves. *Discrete & Continuous Dynamical Systems*, 37(4):2065.
- Pace, S. D., Reiss, K. A., and Campbell, D. K. (2019). The β Fermi-Pasta-Ulam-Tsingou recurrence problem. *Chaos: An Interdisciplinary Journal of Nonlinear Science*, 29(11):113107.
- Schneider, G. and Wayne, C. E. (2000). Counter-propagating waves on fluid surfaces and the continuum limit of the Fermi-Pasta-Ulam model. In *Equadiff 99: (In 2 Volumes)*, pages 390–404. World Scientific.
- Vanderbauwhede, A. and Iooss, G. (1992). Center manifold theory in infinite dimensions. In *Dynamics reported*, pages 125–163. Springer.

Wiggins, S. (1994). *Normally hyperbolic invariant manifolds in dynamical systems*, volume 105. Springer Science & Business Media.