# BOSTON UNIVERSITY COLLEGE OF ARTS AND SCIENCES

### Dissertation

## A BU THESIS LATEX TEMPLATE

by

### TREVOR NORTON

B.S., Virginia Polytechnic Institute and State University, 2015 M.S., Virginia Polytechnic Institute and State University, 2018

Submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy

# Approved by

First Reader	
	First M. Last, PhD Professor of Electrical and Computer Engineering
Second Reader	
	First M. Last Associate Professor of
Third Reader	
	First M. Last Assistant Professor of
Fourth Reader	
	First M. Last Assistant Professor of

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!)

# Acknowledgments

[This is where the acknowledgments go...]

### A BU THESIS LATEX TEMPLATE

### TREVOR NORTON

Boston University, College of Arts and Sciences, 2023

Major Professors: First M. Last, PhD

Professor of Electrical and Computer Engineering

Secondary appointment

First M. Last, PhD

Professor of computer Science

#### ABSTRACT

This is where the text for the abstract will go

# Contents

1 Background Material		kground Material	1
	1.1	Fenichel Theory	1
2 Existence of Kink-Like Travelling Wave Solutions		3	
	2.1	Introduction	3
	2.2	Construction of Center Manifold	5
	2.3	Existence of Heteroclinic Orbit	15
$\mathbf{R}$	efere	nces	19

# List of Abbreviations

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

# Chapter 1

# **Background Material**

### 1.1 Fenichel Theory

(Wiggins, 1994)

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

**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  $\partial M$ .

**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  $h_u(N'^u)$  along  $\overline{M}$  with trajectories in  $W^u(\overline{M})$  approaching  $\overline{M}$  as  $t\to -\infty$ .

**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  $\mathcal{F}^u = \bigcup_{p \in M} f^u(p)$  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

$$\frac{|\phi_{-t}(q) - \phi_{-t}(p)|}{|\phi_{-t}(q) - \phi_{-t}(p)|} \to 0 \quad as \ t \to \infty$$

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.  $\mathcal{F}^u = W^u_{loc}(M)$ .

## Chapter 2

# Existence of Kink-Like Travelling 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

$$u_n(t) = \epsilon \varphi(\epsilon(n+ct)) + \mathcal{O}(\epsilon^3)$$
 (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  $\phi$  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  $\mu$  varies, then one typically has a center manifold containing small bounded parameterized by  $\mu$ . 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  $\epsilon$ , 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  $\phi$ . 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

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

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

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

$$\ddot{x}(t) = \mu \Big( V'(x(t+1) - x(t)) - V(x(t) - x(t-1)) \Big)$$
(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:

$$\partial_t U = L_\mu U + M_\mu(U) \tag{2.5}$$

where  $L_{\mu}$  is the linear operator

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

and

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

$$\mathbb{H} = \mathbb{R}^2 \times C[-1, 1]$$

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

where the spaces have the usual maximum norms. The operator  $L_{\mu}$  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  $L_{\mu_0}$  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:

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

which satisfy

$$L_{\mu_0}\zeta_0 = 0$$

$$L_{\mu_0}\zeta_1 = \zeta_0$$

$$L_{\mu_0}\zeta_2 = \zeta_1$$

$$L_{\mu_0}\zeta_3 = \zeta_2.$$
(2.10)

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

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

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

$$PW = ((PW)_x, (PW)_\xi, (PW)_X)^T$$
  
=  $(PW)_x \zeta_0 + (DW)_x \zeta_1 + (D^2W)_x \zeta_2 + (D^3W)_x \zeta_3$  (2.12)

The projection can be computed by finding the resolvent  $(\lambda I - L_{\mu})^{-1}$  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

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

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

$$X(v) = e^{\lambda v} x - \int_{0}^{v} e^{\lambda(v-s)} F_2(s) ds$$

$$(2.17)$$

with

$$\tilde{f}_{\lambda} = \int_{0}^{1} \left[ -e^{\lambda(1-s)} F_2(s) + e^{-\lambda(1-s)} F_s(-s) \right] ds.$$
 (2.18)

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

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

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

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

$$(D^{2}F)_{x} = (DF)_{\xi} = -12\left(f_{0} - \int_{0}^{1} (1-s)[F_{2}(s) + F_{2}(-s)]ds\right)$$
(2.22)

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

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

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

and we have that

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

where  $\delta_{kj}$  is the Kronecker delta.

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

$$U \mapsto U + q\zeta_0, \quad \forall q \in \mathbb{R}$$
 (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:

$$U = W + q\zeta_0, \quad \zeta_0^*(W) = 0.$$
 (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  $\widehat{L}_{\mu_0}$  acting on  $\mathbb{H}_1$  has the same spectrum as  $L_{\mu_0}$  except that 0 is now a triple eigenvalue instead of a quadruple eigenvalue. One

can check that

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

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

$$W = A\zeta_1 + B\zeta_2 + C\zeta_3 + \Phi_u(A, B, C). \tag{2.31}$$

Here  $\Phi_{\mu}$  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  $\Phi_{\mu}$  (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  $\Phi_{\mu}$  up to a certain order and get an explicit representation of the center manifold (up to some specified error).

We assume that  $\Phi_{\mu}$  can be written as a Taylor series in A, B, C, and  $\mu$ :

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

Note that the  $\mu$  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  $\Phi_{\mu}$  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  $\widehat{L}_{\mu}$  applied to each eigenvector:

$$\widehat{L}_{\mu}\zeta_1 = 0 \tag{2.33}$$

$$\widehat{L}_{\mu}\zeta_{2} = \zeta_{1} + (\mu - 1) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$
(2.34)

$$\widehat{L}_{\mu}\zeta_3 = \zeta_2. \tag{2.35}$$

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

$$\dot{A}\zeta_{1} + \dot{B}\zeta_{2} + \dot{C}\zeta_{3} + D\Phi_{\mu}(A, B, C) \begin{bmatrix} \dot{A} \\ \dot{B} \\ \dot{C} \end{bmatrix} = B\zeta_{1} + B(\mu - 1) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + C\zeta_{3} + L_{\mu_{0}}\Phi_{\mu}(A, B, C) 
+ \left(2(1 - \mu)\Phi_{\mu}^{x} + (\mu - 1)(\delta^{1}\Phi_{\mu}^{X} + \delta^{-1}\Phi_{\mu}^{X})\right) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} 
+ \mu \left(g\left(A + \frac{1}{2}B + \frac{1}{6}C + (\delta^{1}\Phi_{\mu}^{X} - \Phi_{\mu}^{x})\right) - g\left(A - \frac{1}{2}B + \frac{1}{6}C + (\Phi_{\mu}^{x} - \delta^{-1}\Phi_{\mu}^{X})\right)\right) \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$
(2.36)

where we represent the components of  $\Phi_{\mu}$  by  $(\Phi_{\mu}^{x}, \Phi_{\mu}^{\xi}, \Phi_{\mu}^{X})^{T}$ . Now we can group the  $\zeta_{1}, \zeta_{2}$  and  $\zeta_{3}$  together – as well as the remaining terms – to get a system of differential

equations on the center manifold:

$$\dot{A} = B + \frac{2}{5} \left[ \cdots \right] \tag{2.37}$$

$$\dot{B} = C \tag{2.38}$$

$$\dot{C} = -12 \left[ \cdots \right] \tag{2.39}$$

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

The  $\cdots$  within the brackets are given the following expression

$$B(\mu - 1) + 2(1 - \mu)\Phi_{\mu}^{x} + (\mu - 1)(\delta^{1}\Phi_{\mu}^{X} + \delta^{-1}\Phi_{\mu}^{X}) + \mu \left(g\left(A + \frac{1}{2}B + \frac{1}{6}C + (\delta^{1}\Phi_{\mu}^{X} - \Phi_{\mu}^{x})\right) - g\left(A - \frac{1}{2}B + \frac{1}{6}C + (\Phi_{\mu}^{x} - \delta^{-1}\Phi_{\mu}^{X})\right)\right),$$
(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:

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

We will now assume  $\Phi_{\mu}$  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:

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

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

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

Equation (2.45) can be solved by noting that  $\zeta_0$  is the only zero eigenfunction for  $L_{\mu_0}$  and  $\zeta_0^*(\Phi_{100}^{(1)}) = 0$  since  $\Phi_{\mu}$  takes values in  $\mathbb{D}_1$ , thus  $\Phi_{100}^{(1)} = 0$ . Then eq. (2.43) is reduced to

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

which can be solved by integrating to get

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

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

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

with the same value of k.

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

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

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  $\epsilon$ . 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  $\epsilon$ -amplitude waves with wavelength of order  $\epsilon^{-1}$ , we make the following change of variables:

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

Then the equations of motion on the center manifold become

$$\underline{A}' = \underline{B} + \mathcal{O}(\epsilon)$$

$$\underline{B}' = \underline{C}$$

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

Here the  $\mathcal{O}(\epsilon)$  represents functions that are at least  $C^4$  in  $\epsilon$ ,  $\underline{A}$ ,  $\underline{B}$ , and  $\underline{C}$  and can be bounded by a constant times  $\epsilon$  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  $x \to 0$ .

We shall consider two cases going:

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

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

For (1), we have that the flow on the center manifold is given by

$$\underline{A}' = \underline{B} + \epsilon F_1(\underline{A}, \underline{B}, \underline{C}; \epsilon)$$

$$\underline{B}' = \underline{C}$$

$$\underline{C}' = -\underline{B} + 6\underline{A}^2\underline{B} + \epsilon G_1(\underline{A}, \underline{B}, \underline{C}; \epsilon)$$

$$\epsilon' = 0$$
(2.52)

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

$$\underline{A}' = \underline{B} + \eta F_2(\underline{A}, \underline{B}, \underline{C}; \sqrt{\eta})$$

$$\underline{B}' = \underline{C}$$

$$\underline{C}' = -\underline{B} + 6\underline{A}^2\underline{B} + \eta G_2(\underline{A}, \underline{B}, \underline{C}; \sqrt{\eta})$$

$$\eta' = 0$$
(2.53)

where  $F_2$  and  $G_2$  will be  $C^4$  for  $\eta > 0$  and  $\mathcal{O}(1)$  as  $\eta \to 0$ . Reparameterizing to  $\eta$  will ultimately allow us to improve our error from  $\mathcal{O}(\epsilon)$  to  $\mathcal{O}(\epsilon^2)$ . 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

$$\underline{A}''' + \underline{A}' - 6\underline{A}^2\underline{A}' = 0 \tag{2.54}$$

which has the solution

$$\underline{A}(s) = \frac{1}{\sqrt{2}} \tanh\left(\frac{s}{\sqrt{2}}\right). \tag{2.55}$$

This solution is the profile for the kink solution of the defocusing mKdV,  $\phi$ . 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  $s \to \pm \infty$ . 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  $\epsilon$ , and we want to get estimates of these orbits relative to  $\epsilon$ . 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.

We first must find the appropriate overflowing invariant set.<sup>1</sup> From the heteroclinic orbit found for  $\epsilon = 0$ , we know that  $(A, B, C, \epsilon) = (-1/\sqrt{2}, 0, 0, 0)$  should be one point in the set. In fact, for fixed  $\epsilon > 0$  we have that multiples of  $\zeta_1$  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

<sup>1</sup>We need also to find the inflowing invariant set, but we can rely on the symmetry of eq. (2.51)

We 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.

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  $A_0 = -1/\sqrt{2}$ , then

$$\overline{M} = [A_0 - \delta, A_0 + \delta] \times \{0\} \times \{0\} \times [-\epsilon_0, +\epsilon_0]$$
(2.56)

is an invariant set 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 the same. For our case, we may adjust the flow near  $A_0 \pm \delta$  and  $\pm \epsilon_0$  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

$$F_1(\underline{A}, 0, 0, \epsilon) = 0$$

$$G_1(\underline{A}, 0, 0, \epsilon) = 0$$
(2.57)

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

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

$$(2.58)$$

The two eigenvalues  $\lambda_1, \lambda_2 = 0$  correspond with the flow tangent to the manifold. Fixing  $\underline{A} = A_0$  and  $\epsilon = 0$ , the other eigenvalues are  $\lambda_{3,4} = \pm \sqrt{6A_0^2 - 1}$ , which correspond with the flow along the vector bundles  $N^u$  and  $N^s$ , respectively. There at  $p_0 = (A_0, 0, 0, 0)$  we have the generalized Lyapunov-type numbers given by

$$\lambda^{u}(p_0) = e^{-\sqrt{6A_0^2 - 1}}, \quad \nu^{s}(p_0) = e^{-\sqrt{6A_0^2 - 1}}, \quad \sigma^{s}(p_0) = 0.$$
 (2.59)

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  $\delta$  and  $\epsilon_0$  small enough.

# References

- Friesecke, G. and Pego, R. L. (1999). Solitary waves on FPU lattices: I. qualitative properties, renormalization and continuum limit. *Nonlinearity*, 12(6):1601.
- 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 non-linear oscillators. *Communications in Mathematical Physics*, 211(2):439–464.
- Kato, T. (2013). Perturbation theory for linear operators, volume 132. Springer Science & Business Media.
- 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.
- 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.