

BOSTON UNIVERSITY  
COLLEGE OF ARTS AND SCIENCES

Dissertation

**A BU THESIS LATEX TEMPLATE**

by

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

2023



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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!)

## Acknowledgments

[This is where the acknowledgments go...]

# **A BU THESIS LATEX TEMPLATE**

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## **ABSTRACT**

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## List of Abbreviations

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



## Chapter 1

# Existence of Kink-Like Travelling Wave Solutions

### 1.1 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

$$u_n(t) = \epsilon \varphi(\epsilon(n + ct)) + \mathcal{O}(\epsilon^3) \tag{1.1}$$

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. (1.1) 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. (1.1).

## 1.2 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

$$\ddot{x}_n = V'(x_{n+1} - x_n) - V'(x_n - x_{n-1}), \quad n \in \mathbb{Z}. \quad (1.2)$$

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

$$x_n(\tilde{t}) = x(n - c\tilde{t}), \quad (1.3)$$

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

$$\ddot{x}(t) = \mu \left( V'(x(t+1) - x(t)) - V'(x(t) - x(t-1)) \right) \quad (1.4)$$

where  $\mu = c^{-2}$ . Instead of working directly with eq. (1.4), we rewrite the equation as a first-order differential equation in a Banach space. Equation (1.4) 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. (1.4) can be written as follows:

$$\partial_t U = L_\mu U + M_\mu(U) \quad (1.5)$$

where  $L_\mu$  is the linear operator

$$L_\mu = \begin{pmatrix} 0 & 1 & 0 \\ -2\mu & 0 & \mu(\delta^1 + \delta^{-1}) \\ 0 & 0 & \partial_v \end{pmatrix} \quad (1.6)$$

and

$$M_\mu(U) = \mu(0, g(\delta^1 X - x) - g(x - \delta^{-1} X), 0)^T \quad (1.7)$$

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. (1.5) correspond with solutions of eq. (1.4). We introduce the following Banach spaces for  $U$ :

$$\begin{aligned} \mathbb{H} &= \mathbb{R}^2 \times C[-1, 1] \\ \mathbb{D} &= \{U \in \mathbb{R}^2 \times C^1[-1, 1] \mid X(0) = x\} \end{aligned} \quad (1.8)$$

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. (1.5) 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:

$$\begin{aligned} \zeta_0 &= (1, 0, 1)^T & \zeta_1 &= (0, 1, v)^T \\ \zeta_2 &= (0, 0, \frac{1}{2}v^2)^T & \zeta_3 &= (0, 0, \frac{1}{6}v^3)^T \end{aligned} \quad (1.9)$$

which satisfy

$$\begin{aligned}
L_{\mu_0}\zeta_0 &= 0 \\
L_{\mu_0}\zeta_1 &= \zeta_0 \\
L_{\mu_0}\zeta_2 &= \zeta_1 \\
L_{\mu_0}\zeta_3 &= \zeta_2.
\end{aligned} \tag{1.10}$$

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

$$(\lambda I - L_{\mu_0})^{-1} = \frac{D^3}{\lambda^4} + \frac{D^2}{\lambda^2} + \frac{D}{\lambda^2} + \frac{P}{\lambda} - \tilde{L}_{\mu_0}^{-1} + \lambda \tilde{L}_{\mu_0}^{-1} - \dots \tag{1.11}$$

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

$$\begin{aligned}
PW &= ((PW)_x, (PW)_\xi, (PW)_X)^T \\
&= (PW)_x\zeta_0 + (DW)_x\zeta_1 + (D^2W)_x\zeta_2 + (D^3W)_x\zeta_3
\end{aligned} \tag{1.12}$$

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

$$(\lambda I - L_\mu)U = F. \tag{1.13}$$

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

$$N(\lambda; \mu) = -\lambda^2 + 2\mu(\cosh \lambda - 1) \tag{1.14}$$

and  $U$  is given by

$$x = -[N(\lambda; \mu)]^{-1}(\lambda f_0 + f_1 + \mu \tilde{f}_\lambda) \quad (1.15)$$

$$\xi = -[N(\lambda; \mu)]^{-1}([\lambda^2 + N(\lambda; \mu)]f_0 + \lambda f_1 + \mu \lambda \tilde{f}_\lambda) \quad (1.16)$$

$$X(v) = e^{\lambda v} x - \int_0^v e^{\lambda(v-s)} F_2(s) ds \quad (1.17)$$

with

$$\tilde{f}_\lambda = \int_0^1 [-e^{\lambda(1-s)} F_2(s) + e^{-\lambda(1-s)} F_s(-s)] ds. \quad (1.18)$$

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

$$(PF)_x = \text{Res}((\lambda I - L_{\mu_0}^{-1} F)_x, 0) = \text{Res}(-[N(\lambda; \mu)]^{-1}(\lambda f_0 + f_1 + \mu \tilde{f}_\lambda), 0). \quad (1.19)$$

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

$$(PF)_x = \frac{2}{5} \left( f_0 - \int_0^1 [(1-s) - 5(1-s)^3][F_2(s) + F_2(-s)] ds \right) \quad (1.20)$$

$$(DF)_x = (PF)_\xi = \frac{2}{5} \left( f_1 - \int_0^1 [1 - 15(1-s)^2][F_2(s) - F_2(-s)] ds \right) \quad (1.21)$$

$$(D^2 F)_x = (DF)_\xi = -12 \left( f_0 - \int_0^1 (1-s)[F_2(s) + F_2(-s)] ds \right) \quad (1.22)$$

$$(D^3 F)_x = (D^2 F)_\xi = -12 \left( f_1 - \int_0^1 [F_2(s) - F_2(-s)] ds \right). \quad (1.23)$$

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

$$\begin{aligned}\zeta_0^*(F) &= (PF)_x \\ \zeta_1^*(F) &= (DF)_x = \zeta_0^*(L_{\mu_0}F) \\ \zeta_2^*(F) &= (D^2F)_x \\ \zeta_3^*(F) &= (D^3F)_x\end{aligned}\tag{1.24}$$

and we have that

$$\zeta_k^*(\zeta_j) = \delta_{kj} \quad k, j = 0, 1, 2, 3 \tag{1.25}$$

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. (1.5) is invariant under

$$U \mapsto U + q\zeta_0, \quad \forall q \in \mathbb{R} \tag{1.26}$$

which corresponds to the shift invariance of eq. (1.4). This invariance allows us to reduce the center manifold to a three-dimensional manifold. We first decompose  $U \in \mathbb{H}$  as follows:

$$U = W + q\zeta_0, \quad \zeta_0^*(W) = 0. \tag{1.27}$$

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. (1.5) becomes

$$\frac{dq}{dt} = \zeta_0^*(L_\mu W) = \zeta_0^*(L_{\mu_0} W) = \zeta_1^*(W) \tag{1.28}$$

$$\frac{dW}{dt} = \widehat{L}_\mu W + M_\mu(W) \tag{1.29}$$

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.

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

by

$$W = A\zeta_1 + B\zeta_2 + C\zeta_3 + \Phi_\mu(A, B, C). \quad (1.30)$$

Here  $\Phi_\mu$  takes values in  $\mathbb{D}_1$ . Note that this implies solutions on the center manifold correspond with solutions of eq. (1.4), 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  $\mu$ :

$$\Phi_\mu(A, B, C) = \sum_{i,j,k,\ell} (\mu - 1)^\ell A^i B^j C^k \Phi_{ijk}^{(\ell)} \quad (1.31)$$

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. (1.31). 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  $g$ .

### 1.3 Existence of Heteroclinic Orbit



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