

The cover features an abstract graphic design. In the top left, there are blue shapes consisting of a cluster of small circles and larger, rounded, overlapping forms. In the top right, there are white shapes, including a horizontal row of circles and larger, rounded, overlapping forms. The background is dark with a blurred, fiery orange and red circular pattern in the center.

Alexander Pankov

**Travelling Waves and Periodic  
Oscillations in Fermi-Pasta-  
Ulam Lattices**

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# Travelling Waves and Periodic Oscillations in Fermi-Pasta- Ulam Lattices

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**TRAVELLING WAVES AND PERIODIC OSCILLATIONS  
IN FERMI – PASTA – ULAM**

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**Travelling Waves and Periodic  
Oscillations in Fermi-Pasta-  
Ulam Lattices**

To Tanya

# Preface

In the past two decades, there has been an explosion of interest to the study of wave propagation in spatially discrete nonlinear systems.

Probably, the most prominent example of such a system is the famous Fermi-Pasta-Ulam (FPU) lattice introduced in the pioneering work [Fermi *et. al* (1955)]. E. Fermi, J. Pasta and S. Ulam studied numerically the lattices of identical particles, *i. e.* monoatomic lattices, with cubic and quartic interaction potentials. These lattices are known today as  $\alpha$ - and  $\beta$ -models, respectively. The aim of E. Fermi, J. Pasta and S. Ulam was to show the relaxation to equipartition of the distribution of energy among modes. Surprisingly enough, their numerical simulation yielded the opposite result. They observed that, at least at low energy, the energy of the system remained confined among the initial modes, instead of spreading towards all modes.

This work motivated a great number of further numerical and analytical investigations (for a relatively recent survey of the subject see [Poggi and Ruffo (1997)]). We mention here the so-called Toda lattice which is a completely integrable system. Due to the integrability, the dynamics of Toda lattice is well-understood (see [Toda (1989); Teschl (2000)]). Unfortunately, the Toda lattice is the only known completely integrable lattice of FPU type. Overwhelming majority of existing results concern either particular explicit solutions, both exact and approximate, or numerical simulation. Moreover, almost exclusively spatially homogeneous, *i. e.* monoatomic, lattices are under consideration, although inhomogeneous lattices (multiatomic lattices, lattices with impurities, *etc.*) are of great interest.

One of the first rigorous results about general FPU type lattices was

obtained in [Friesecke and Wattis (1994)]. G. Friesecke and J. Wattis have proved the existence of solitary travelling waves in monoatomic FPU lattices under some general assumptions on the potential of interparticle interaction. The class of potentials includes the  $\alpha$ - and  $\beta$ - models, the Toda potential, the Lennard-Jones potential, and others. The approach of G. Friesecke and J. Wattis is based on an appropriate constrained minimization procedure and the concentration compactness principle of P.-L. Lions [Lions (1984)]. In this approach the wave speed is unknown and is determined *a posteriori* through the corresponding Lagrange multiplier.

Later on D. Smets and M. Willem [Smets and Willem (1997)] considered the travelling wave problem as a problem with *prescribed* speed. Under another set of assumptions they have proved the existence of travelling waves for every prescribed speed beyond the speed of sound (naturally defined). The proof relies upon an appropriate version of the mountain pass theorem without Palais-Smale condition. In [Pankov and Pflüger (2000b)], K. Pflüger and the author revised the last approach considerably choosing periodic travelling waves as a starting point. The existence of periodic waves is obtained by means of the standard mountain pass theorem. Then one gets solitary waves in the limit as the wave lengths goes to infinity. This approach applies to many other problems (see, *e. g.* [Pankov and Pflüger (1999); Pankov and Pflüger (2000a)]).

We mention also the series of papers [Friesecke and Pego (1999); Friesecke and Pego (2002); Friesecke and Pego (2004a); Friesecke and Pego (2004b)], where near sonic solitary waves are studied. Under some generic assumptions on the potential of interaction near the origin the existence of such waves is obtained by means of perturbation from the standard Korteweg-de Vries (KdV) soliton. Many properties of near sonic waves are discussed including their dynamical stability.

Another line of development was originated by B. Ruf and P. Srikanth [Ruf and Srikanth (1994)] who considered time periodic motions of finite FPU type lattices not necessary consisting of identical particles. Similar problem for infinite lattices, still inhomogeneous, was studied in [Arioli and Chabrowski (1997); Arioli and Gazzola (1995); Arioli and Gazzola (1996); Arioli *et. al* (1996); Arioli and Szulkin (1997)] under more restrictive assumptions on the potential.

Another class of discrete media consists of chains of coupled nonlinear oscillators. One of the most known models of such kind is the so-called

Frenkel-Kontorova model introduced by Ya. Frenkel and T. Kontorova in 1938. As we have learned from [Braun and Kivshar (2004)], the same model have been appeared even before, in works by L. Prandtl and U. Dehlinger (1928–29). For physical applications of the Frenkel-Kontorova and related models we refer to [Braun and Kivshar (1998)] and [Braun and Kivshar (2004)]. Also chains of oscillators as systems that support breathers, *i. e.* spatially localized time periodic solutions, were studied in many works (see [Aubry (1997); James (2003); Livi *et. al* (1997); MacKay and Aubry (1994); Morgante *et. al* (2002)] and references therein). Some other mathematical results that concern time periodic solutions and travelling waves in such systems can be found in [Bak (2004); Bak and Pankov (2004); Bak and Pankov (to appear); Iooss and Kirschgässner (2000)].

Finally, we mention the third class of discrete systems of common interest – discrete nonlinear Schrödinger equations. Such equations are not considered here (see [Flach and Willis (1998); Hennig and Tsironis (1999); Kevrekidis and Weinstein (2003); Pankov and Zakharchenko (2001); Weinstein (1999)] and references therein).

## Contents

The main aim of this book is to present rigorous results on time periodic oscillations and travelling waves in FPU lattices. Also we consider briefly similar results for chains of oscillators. Actually, we confine ourself in the circle of the results obtained by variational methods. Therefore, other approaches, like bifurcation theory and perturbation analysis, are not presented here. As we mentioned before, discrete nonlinear Schrödinger equations are outside the scope of the book.

In Chapter 1 we discuss general properties of equations that govern the dynamics of FPU lattices and chains of oscillators, with special attention paid to the well-posedness of the Cauchy problem. Also we remind here basic facts from the spectral theory of linear difference operators that are relevant to linear FPU lattices.

Chapter 2 deals with the existence of time periodic solutions in the lattices of FPU type. Since we employ global variational techniques, it is not natural to restrict the analysis to the case of spatially homogeneous, *i. e.* monoatomic, lattices. Instead, we allow periodic spatial inhomogeneities that means that we consider regular multiatomic lattices. We give complete proofs of all principal results. At the same time, for the results that



require more technicalities we outline basic ideas and skip details. Also, skipping technical details, we present couple of results on the existence of time periodic solutions in some chains of nonlinear oscillators.

In Chapters 3 and 4 we study travelling waves in monoatomic FPU lattices. The first of them is devoted to waves with prescribed speed. This statement of problem seems to be most natural. Here we consider two types of travelling waves, periodic and solitary. In fact, we treat solitary waves as a limit case of periodic waves when the wavelength goes to infinity. In Chapter 4 we give some additional results. First of all, we present in details the approach of G. Friesecke and J. Wattis. This approach is technically more involved and, therefore, is postponed to the last chapter. Also we discuss here several other results, including exponential decay of solitary waves, as well as travelling waves in chains of oscillators.

Each chapter, except Chapter 3, ends with a special section devoted to various comments and open problems. Comments and open problems that concern travelling waves are put on the end of Chapter 4. Open problems we offer reflect author's point of view on what should be done next. Some of them are accessible by existing methods, while others are probably hard enough.

For reader's convenience we include four appendices. Their aim is to remind basic facts about functional spaces, concentration compactness, critical points and finite differences, and make the presentation more or less self-contained.

### **Audience**

As audience we have researchers in mind. Although the book is formally self-contained, some acquaintance with variational methods and nonlinear analysis is recommended. Appropriate references are [Mawhin and Willem (1989); Rabinowitz (1986); Struwe (2000); Willem (1996)] (variational methods) and [Zeidler (1995a); Zeidler (1995b)] (nonlinear analysis). At the same time the present book is accessible to graduate students as well, especially in combinations with the books on variational methods listed above.

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A. Pankov

# Contents

<i>Preface</i>	vii
1. Infinite Lattice Systems	1
1.1 Equations of motion . . . . .	1
1.2 The Cauchy problem . . . . .	7
1.3 Harmonic lattices . . . . .	10
1.4 Chains of coupled nonlinear oscillators . . . . .	16
1.5 Comments and open problems . . . . .	24
2. Time Periodic Oscillations	27
2.1 Setting of problem . . . . .	27
2.2 Positive definite case . . . . .	34
2.3 Indefinite case . . . . .	42
2.3.1 Main result . . . . .	42
2.3.2 Periodic approximations . . . . .	46
2.3.3 Proof of main result . . . . .	54
2.4 Additional results . . . . .	56
2.4.1 Degenerate case . . . . .	56
2.4.2 Constrained minimization . . . . .	58
2.4.3 Multibumps . . . . .	59
2.4.4 Lattices without spatial periodicity . . . . .	61
2.4.5 Finite lattices . . . . .	62
2.5 Chains of oscillators . . . . .	64
2.6 Comments and open problems . . . . .	70
3. Travelling Waves: Waves with Prescribed Speed	75

3.1	Statement of problem . . . . .	75
3.2	Periodic waves . . . . .	78
3.2.1	Variational setting . . . . .	78
3.2.2	Monotone waves . . . . .	81
3.2.3	Nonmonotone and subsonic waves . . . . .	85
3.3	Solitary waves . . . . .	89
3.3.1	Variational statement of the problem . . . . .	89
3.3.2	From periodic waves to solitary ones . . . . .	93
3.3.3	Global structure of periodic waves . . . . .	101
3.3.4	Examples . . . . .	104
3.4	Ground waves: existence and convergence . . . . .	105
3.4.1	Ground waves: periodic case . . . . .	105
3.4.2	Solitary ground waves . . . . .	109
3.4.3	Monotonicity . . . . .	112
3.5	Near sonic waves . . . . .	114
3.5.1	Amplitude estimate . . . . .	114
3.5.2	Nonglobally defined potentials . . . . .	117
4.	Travelling Waves: Further Results . . . . .	121
4.1	Solitary waves and constrained minimization . . . . .	121
4.1.1	Statement of problem . . . . .	121
4.1.2	The minimization problem: technical results . . . . .	123
4.1.3	The minimization problem: existence . . . . .	133
4.1.4	Proof of main result . . . . .	140
4.1.5	Lennard-Jones type potentials . . . . .	143
4.2	Other types of travelling waves . . . . .	146
4.2.1	Waves with periodic profile functions . . . . .	146
4.2.2	Solitary waves whose profiles vanish at infinity . . . . .	148
4.3	Yet another constrained minimization problem . . . . .	150
4.4	Remark on FPU $\beta$ -model . . . . .	152
4.5	Exponential decay . . . . .	154
4.6	Travelling waves in chains of oscillators . . . . .	160
4.7	Comments and open problems . . . . .	163
	Appendix A Functional Spaces . . . . .	167
	A.1 Spaces of sequences . . . . .	167
	A.2 Spaces of functions on real line . . . . .	168
	Appendix B Concentration Compactness . . . . .	173

Appendix C	Critical Point Theory	177
C.1	Differentiable functionals . . . . .	177
C.2	Mountain pass theorem . . . . .	178
C.3	Linking theorems . . . . .	179
Appendix D	Difference Calculus	183
<i>Bibliography</i>		185
<i>Index</i>		193

# Chapter 1

## Infinite Lattice Systems

### 1.1 Equations of motion

We consider a one dimensional chain of particles with nearest neighbor interaction. Equations of motion of the system read

$$m(n)\ddot{q}(n) = U'_{n+1}(q(n+1) - q(n)) - U'_n(q(n) - q(n-1)), \quad n \in \mathbb{Z}. \quad (1.1)$$

Here  $q(n) = q(t, n)$  is the coordinate of  $n$ -th particle at time  $t$ ,  $m(n)$  is the mass of that particle, and  $U_n$  is the potential of interaction between  $n$ -th and  $(n-1)$ -th particles. We always assume that there are positive constants  $m_0$  and  $M_0$  such that

$$m_0 \leq m(n) \leq M_0$$

for every  $n \in \mathbb{Z}$ .

Equations (1.1) form an infinite system of ordinary differential equations which is a Hamiltonian system with the Hamiltonian

$$H = \sum_{n=-\infty}^{\infty} \left( \frac{p^2(n)}{2m(n)} + U_n(q(n+1) - q(n)) \right), \quad (1.2)$$

where  $p(n) = m(n)\dot{q}(n)$  is the momentum of  $n$ -th particle.

Formally this statement is readily verified. However, to make it precise first one has to specify the phase space.

The simplest, but not so natural from the point of view of physics, choice of the configuration space is the space  $l^2$  of two-sided sequences<sup>1</sup>

---

<sup>1</sup>For the definitions and notations of spaces of sequences see Appendix A.1.

$q = \{q(n)\}_{n \in \mathbb{Z}}$ . This corresponds to the boundary condition

$$\lim_{n \rightarrow \pm\infty} q(n) = 0 \quad (1.3)$$

at infinity.

In this case the phase space is  $l^2 \times l^2$  and Eq. (1.1) can be written as the first-order system

$$\dot{u} = J \nabla H(u),$$

where

$$u = \begin{pmatrix} q \\ p \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} : l^2 \times l^2 \rightarrow l^2 \times l^2,$$

$I$  is the identity operator and  $\nabla H$  the functional gradient of  $H$

$$\nabla H(u)(n) = \begin{pmatrix} U'_n(q(n) - q(n-1)) - U'_{n+1}(q(n+1) - q(n)) \\ p(n)/m(n) \end{pmatrix}.$$

Denote by  $G$  the nonlinear operator defined by

$$G(q)(n) = U'_n(q(n)), \quad n \in \mathbb{Z}, \quad (1.4)$$

where  $q = \{q(n)\}$ , and consider operators of right and left differences

$$(\partial^+ q)(n) := q(n+1) - q(n)$$

and

$$(\partial^- q)(n) := q(n) - q(n-1),$$

respectively. We suppose that  $G$  is a “good” nonlinear operator in  $l^2$ . Then

$$\nabla H(u) = \begin{pmatrix} -\partial^+ G(\partial^- q) \\ p/m \end{pmatrix}, \quad (1.5)$$

while Eq. (1.1) becomes a “divergence form” equation

$$m\ddot{q} = \partial^+ G(\partial^- q). \quad (1.6)$$

Note that  $\partial^+$  and  $\partial^-$  are bounded linear operators in  $l^2$  and

$$(\partial^+)^* = -\partial^-.$$

Another form of Eq. (1.6) is

$$m\ddot{q} = \partial^- G^+(\partial^+ q), \quad (1.7)$$

where

$$G^+(q)(n) = U'_{n+1}(q(n)). \quad (1.8)$$

However, more natural and most important choice of configuration space is the space  $X = \tilde{l}^2$  that consists of two-sided sequences  $q = \{q(n)\}_{n \in \mathbb{Z}}$  such that  $\partial^+ q \in l^2$ . Endowed with the norm

$$\|q\|_X = (\|\partial^+ q\|_{l^2}^2 + |q(0)|^2)^{1/2} = (\|\partial^- q\|_{l^2}^2 + |q(0)|^2)^{1/2},$$

$X$  is a Hilbert space. Obviously,

$$\|\partial^- q\|_{l^2} = \|\partial^+ q\|_{l^2}.$$

Operators  $\partial^+$  and  $\partial^-$  are linear bounded operators from the space  $X$  onto  $l^2$  and have one dimensional kernel that consists of constant sequences.

Equation (1.1) (equivalently, (1.6)) is a Hamiltonian system on the phase space  $\tilde{l}^2 \times l^2$ . In this case the corresponding symplectic form [Marsden and Ratiu (1994)] is degenerate. Nevertheless, the Hamiltonian  $H$  defined by (1.2) is a conserved quantity provided  $H(q, p)$  is  $C^1$  on  $\tilde{l}^2 \times l^2$ . This can be verified by a direct calculation.

Now we introduce a reformulation of Eq. (1.6) in  $\tilde{l}^2$  as an equation in  $l^2$ . Denote by

$$r(n) := q(n+1) - q(n),$$

i. e.  $r = \partial^+ q$ , the *relative displacements* of adjacent lattice sites and set

$$b(n) := a(n-1) = m(n)^{-1/2}.$$

Then Eq. (1.1) gives immediately

$$\begin{aligned} \ddot{r}(n) &= a^2(n) [U'_{n+1}(r(n+1)) - U'_n(r(n))] \\ &\quad - a^2(n-1) [U'_n(r(n)) - U'_{n-1}(r(n-1))]. \end{aligned} \quad (1.9)$$

Note that  $r \in l^2$  whenever  $q \in \tilde{l}^2$ . In operator form, Eq.(1.9) reads

$$\ddot{r} = \partial^- [a^2 \partial^+ G(r)].$$

Also it can be written as (see Appendix D, Eq. (D.5))

$$\ddot{r} = \partial^+ [b^2 \partial^- G^+(r)], \quad (1.10)$$



where

$$G^+(r)(n) = U'_{n+1}(r(n)).$$

Equation (1.10) is equivalent to the following first-order system

$$\dot{u} = F(u), \quad u = \begin{pmatrix} r \\ s \end{pmatrix}, \quad F(u) = \begin{pmatrix} \partial^+(bs) \\ b\partial^-G^+(r) \end{pmatrix}. \quad (1.11)$$

This is a Hamiltonian system

$$\dot{u} = J\nabla H(u), \quad (1.12)$$

where

$$J = \begin{pmatrix} 0 & \partial^+b \\ -b\partial^- & 0 \end{pmatrix} \quad (1.13)$$

and

$$H(r, s) = \sum_{n=-\infty}^{\infty} \left[ \frac{s(n)^2}{2} + U_{n+1}(r(n)) \right]. \quad (1.14)$$

In fact, here  $s = bp = p/m^{1/2}$ . The phase space of this system is  $l^2 \times l^2$ . It is readily verified that

$$(\partial^+b)^* = -b\partial^-.$$

Certainly,  $H(r, s)$  defined by (1.14) is a conserved quantity if  $H$  is  $C^1$  on  $l^2 \times l^2$ .

Now let us discuss the relation between solutions of Eq. (1.6) and Eq. (1.10) (or (1.11)). Consider a solution  $q = q(t, n)$  of Eq. (1.6) such that  $q$  is a  $C^1$  function of  $t$  with values in  $X = \tilde{l}^2$  and  $\dot{q}$  is a  $C^1$  function with values in  $l^2$ . Then  $r = \partial^+q$  and  $s = ap$  are  $C^1$  functions with values in  $l^2$ , and  $u = (r, s)$  obviously solves (1.11). Moreover, the well-posedness, local or global in time, of the Cauchy problem for Eq. (1.6) in  $\tilde{l}^2 \times l^2$  implies the same property for Eq. (1.11) (and (1.10)) in the space  $l^2 \times l^2$ .

Conversely, consider the Cauchy problem for (1.6), with

$$q|_{t=0} = q^{(0)} \in \tilde{l}^2, \quad \dot{q}|_{t=0} = q^{(1)} \in l^2.$$

Set

$$r^{(0)} = \partial^+q^{(0)}, \quad s^{(0)} = m^{1/2}q^{(1)}.$$