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

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

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

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

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

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

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[1]

[1] 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

$$\lim_{n\to\pm\infty} q(n) = 0 \tag{1.3}$$

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

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

I is the identity operator and ∇H the functional gradient of H

$$\nabla H(u)(n) = \begin{pmatrix} U_n'\big(q(n) - q(n-1)\big) - U_{n+1}'\big(q(n+1) - q(n)\big) \\ p(n)/m(n) \end{pmatrix}.$$

Denote by G the nonlinear operator defined by

$$G(q)(n) = U_n'\big(q(n)\big), \quad n \in \mathbb{Z}, \tag{1.4}$$

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

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

while Eq. (1.1) becomes a "divergence form" equation

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

Note that ∂^+ and ∂^- are bounded linear operators in l^2 and

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

Another form of Eq. (1.6) is

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

where

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

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

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

X is a Hilbert space. Obviously,

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

Operators ∂^+ and ∂^- 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 $\widetilde{l^2} \times l^2$. 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 $\widetilde{l^2} \times l^2$. This can be verified by a direct calculation.

Now we introduce a reformulation of Eq. (1.6) in $\widetilde{l^2}$ 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

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

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

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

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

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

where

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

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

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

This is a Hamiltonian system

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

where

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

and

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

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 $X = \widetilde{l^2}$ 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 $\widetilde{l^2} \times l^2$ 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

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

Set

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

Let $u = (r, s)$ be the solution of Cauchy problem for Eq. (1.11), with

$$u|_{t=0} = \left(r^{(0)}, s^{(0)}\right) \in l^2 \times l^2.$$

Define

$$q(t) = q^{(0)} + \int_0^t bs(\tau)\, d\tau.$$

Equation (1.11) implies that $\partial^+ q = r$. We have $\dot{q} = bs$ and, by Eq. (1.11),

$$\ddot{q} = b\dot{s} = b^2 \partial^- G^+(r) = b^2 \partial^- G^+(\partial^+ q).$$

Hence,

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

which is another form (1.7) of Eq. (1.6). Obviously $\dot{q}|_{t=0} = q^{(1)}$. Thus, the two statements of problem, (1.6) and (1.11), are equivalent.

Now let us consider several examples. In these examples we always have $m(n) \equiv 1$, $U_n(r) \equiv U(r)$.

Example 1.1 Let

$$U(r) = \frac{c_0}{2} r^2, \quad c_0 > 0.$$

Then we obtain the *discrete wave equation*

$$\ddot{q} = c_0 \Delta q, \tag{1.15}$$

where $\Delta = \partial^+ \partial^-$ is the *discrete one-dimensional Laplacian.*

Example 1.2 If

$$U(r) = \frac{c_0}{2} r^2 + \frac{c_1}{3} r^3, \quad c_0 > 0, \quad c_1 \neq 0,$$

(cubic interaction), we obtain the so-called *Fermi-Pasta-Ulam α-model.*

Example 1.3 The *Fermi-Pasta-Ulam β-model* is defined by

$$U(r) = \frac{c_0}{2} r^2 + \frac{c_2}{4} r^4, \quad c_0 > 0, \quad c_2 > 0$$

(quartic interaction).

Example 1.4 The well-known *Toda lattice* [Toda (1989)] has the potential of interaction

$$U(r) = ab^{-1}(e^{-br} + br - 1).$$

This is an example of completely integrable Hamiltonian system [Toda (1989); Teschl (2000)].

Example 1.5 The *Lennard-Jones potential* [Friesecke and Wattis (1994)] is a singular potential defined by

$$U(r) = a\big[(d+r)^{-12} - 2d^{-6}(d+r)^{-6} + d^{-12}\big] = a\big[(d+r)^{-6} - d^{-6}\big]^2, \quad r > -d.$$

More generally, one considers the potentials

$$U(r) = a\big[(d+r)^{-k} - d^{-k}\big]^2,$$

with $a > 0$, $d > 0$ and positive integer k [Friesecke and Matthies (2002)].

In classical FPU lattices $m(n) \equiv m_0$ and U_n does not depend on $n \in \mathbb{Z}$. Such lattices are often called *monoatomic* lattices. More general class of FPU type lattices consists of systems with periodic dependence of $m(n)$ and U_n on $n \in \mathbb{Z}$, *i. e.* $m(n+N) = m(n)$, $U_{n+N} = U_n$. This is the class of *multiatomic*, or *N-atomic* lattices. If $N = 2$, such systems are called *diatomic* lattices.

Another interesting class of FPU type systems, *lattices with impurities*, appears when we assume that $m(n)$ and U_n are close to periodic for large values of $|n|$, *i. e.* $m = \overline{m} + m^{(0)}$ and $U_n(r) = \overline{U}_n(r) + U_n^{(0)}(r)$, where $\overline{m}(n)$ and $\overline{U}_n$ are N-periodic in n, while

$$\lim_{|n|\to\infty} m^{(0)}(n) = 0,$$

$$\lim_{|n|\to\infty} U_n^{(0)}(r) = 0.$$

In particular, if $m^{(0)}(n)$ and $U_n^{(0)}$ vanish for all, but finite, values of n, such a system can be viewed as a multiatomic lattice perturbed by replacing a finite number of original particles by particles of another sort, *i. e.* introducing an impurity.

1.2 The Cauchy problem

Consider the Cauchy problem for Eq. (1.12) or, equivalently, for Eq. (1.13) with the data

$$r|_{t=0} = r^{(0)} \in l^2, \quad \dot{r}|_{t=0} = r^{(1)} \in l^2, \tag{1.16}$$

or, respectively,

$$u|_{t=0} = u^{(0)} = \left(r^{(0)}, s^{(0)}\right) \in l^2 \times l^2. \tag{1.17}$$

We impose the following assumptions.

(*i*) *There exist* $M_0 \geq m_0 \geq 0$ *such that*

$$m_0 \leq m(n) \leq M_0, \quad n \in \mathbb{Z}.$$

(*ii*) *The potential* $U_n(r)$ *is a* C^1 *function on* $\mathbb{R}$, $U_n(0) = U_n'(0) = 0$ *and for every* R *there exists* $C(R) > 0$ *such that for all* $n \in \mathbb{Z}$

$$\left|U_n'(r_1) - U_n'(r_2)\right| \leq C(R)\,|r_1 - r_2|, \quad |r_1|, |r_2| \leq R. \tag{1.18}$$

Lemma 1.1 *Under assumption (ii) the operators* G *and* G^+ *(see Eqs. (1.4) and (1.8)) act in* l^2 *and are bounded locally Lipschitz continuous operators, i. e.*

$$\left\|G(q^{(1)}) - G(q^{(2)})\right\|_{l^2} \leq C(R)\,\|q^{(1)} - q^{(2)}\|_{l^2}, \quad \|q^{(1)}\|_{l^2}, \|q^{(2)}\|_{l^2} \leq R,$$

and similar inequalities for G^+.

Proof. Let $q \in l^2$ and $\|q\|_{l^2} \leq R$. Then $\|q\|_{l^\infty} \leq R$ and (1.18) implies that

$$\|G(q)\|_{l^2} \leq C\left(\|q\|_{l^\infty}\right) \|q\|_{l^2} \leq C(R)\,\|q\|_{l^2}.$$

Hence, G acts from l^2 into itself. The remaining parts of the lemma are similar. □

Since $b = m^{-1/2}$ is a bounded sequence and the operators ∂^+ and ∂^- are bounded in l^2, the operator F in (1.11) acts from $l^2 \times l^2$ into itself and is a bounded locally Lipschitz continuous operator in that space. Therefore, the standard infinite dimensional version of the classical Picard theorem (see, *e. g.*, [Dalec'kii and Krein (1974); Zeidler (1986); Zeidler (1995b)]) implies the following local well-posedness result

Theorem 1.1 *Under assumptions (i) and (ii), for every*

$$u^{(0)} = \left(r^{(0)}, s^{(0)}\right) \in l^2 \times l^2$$

there exists a unique solution

$$u = (r, s) \in C^1\left((-a, a), l^2 \times l^2\right)$$

of problem (1.13), (1.17). For any ball $B \subset l^2 \times l^2$ of initial data $u^{(0)}$ the number $a \in \mathbb{R}$ can be chosen independent on $u^{(0)}$ and for every $a' \in (0, a)$ the solution u as an element of $C^1\left([-a', a'], l^2 \times l^2\right)$ depends continuously on the initial data $u^{(0)} \in B$.

The problem of global existence is more delicate. A simple result of such kind is

Theorem 1.2 *Suppose that assumptions (i) and (ii), with (1.18) replaced by stronger inequality*

$$\left|U_n'(r_1) - U_n'(r_2)\right| \leq C\left|r_1 - r_2\right|, \quad r_1, r_2 \in \mathbb{R}, \tag{1.19}$$

are satisfied. Then for every $u^{(0)} \in l^2 \times l^2$ problem (1.13), (1.17) has a unique solution defined on $\mathbb{R}$.

This theorem is a particular case of a well-known result (see, *e. g.*, [Dalec'kii and Krein (1974)], Theorem 1.2 of Chapter 8). However, it has a limited range of applications, since Eq. (1.19) means in particular that the potential U_n has at most quadratic growth at infinity.

Theorem 1.3 *Suppose that assumptions (i) and (ii) are satisfied and either*

(a) $U_n(r) \geq 0$ for all $n \in \mathbb{Z}$ and $r \in \mathbb{R}$,

or

(b) there exists a nondecreasing continuous function $h(r)$, $r \geq 0$, such that $\lim_{r\to\infty} h(r) = +\infty$ and for every $n \in \mathbb{Z}$

$$U_n(r) \geq h\left(|r|\right), \quad r \in \mathbb{R}.$$

Then for every $u^{(0)} = \left(r^{(0)}, s^{(0)}\right) \in l^2 \times l^2$ Cauchy problem (1.13), (1.17) has a unique global solution, i. e. solution defined for all $t \in \mathbb{R}$.

Proof. It is readily verified that the Hamiltonian $H(r,s)$ defined by Eq. (1.14) is a C^1 functional on $l^2 \times l^2$ and, hence, a conserved quantity. Thus, for any solution $u(t) = \big(r(t), s(t)\big)$ of problem (1.13), (1.17)

$$H\big(r(t), s(t)\big) = H\big(r^{(0)}, s^{(0)}\big).$$

In case (a) this implies that

$$\frac{1}{2}\,\|s(t)\|^2 \leq H\big(r^{(0)}, s^{(0)}\big).$$

Since $\dot{r} = \partial^+(bs)$, we obtain by integration that $\|r(t)\|$ remains bounded on any finite interval of existence of solution. This is enough to conclude that the solution is defined everywhere on $\mathbb{R}$ (see, *e. g.*, [Reed and Simon (1975)], Theorem X.74).

Now we consider case (b). Fix $H_0 \geq 0$ such that $H\big(r^{(0)}, s^{(0)}\big) \leq H_0$. Conservation of the Hamiltonian implies that

$$\frac{1}{2}\,s(t,n)^2 + h\big(|r(t,n)|\big) \leq H_0.$$

Let $\overline{r} > 0$ be a solution of the equation

$$h(\overline{r}) = H_0.$$

Obviously, such a solution exists. Then $|r(t,n)| \leq \overline{r}$.

Now we introduce a modified potential defined as follows. Let $\psi(r)$ be an even function such that

$$\psi(r) = \begin{cases} 1 & \text{if} \quad 0 \leq r \leq \overline{r}, \\ -r + \overline{r} + 1 & \text{if} \quad \overline{r} \leq r \leq \overline{r} + 1, \\ 0 & \text{if} \quad r \geq \overline{r}. \end{cases}$$

Define $\widetilde{U}_n(r)$ by the formula

$$\widetilde{U}_n(r) = \int_0^r \Big[\psi(\varrho)\, U_n'(\varrho) + \big(1 - \psi(\varrho)\big)\varrho\Big]\, d\varrho.$$

It is a simple exercise to verify that $\widetilde{U}_n$ satisfies assumption (1.19). Hence, the modified Hamiltonian satisfies the assumptions of Theorem 1.2. On the solution $u(t) = \big(r(t), s(t)\big)$, $\widetilde{H}$ coincides with H. Therefore, $u(t)$ extends to a global solution of the modified system. An elementary, but somewhat long, calculation shows that $\widetilde{U}_n(r) \geq \widetilde{h}(|r|)$, where

$$\widetilde{h}(r) = \begin{cases} h(r), & 0 \leq r \leq \bar{r}, \\ (\bar{r}+1-r)\,h(r) + \displaystyle\int_{\bar{r}}^{r} h(\varrho)\,d\varrho + \left(\frac{r^3}{3} - \bar{r}\frac{r^2}{2} + \frac{\bar{r}^3}{6}\right), & \bar{r} \leq r \leq \bar{r}+1, \\ r^2 + \displaystyle\int_{\bar{r}}^{\bar{r}+1} h(\varrho)\,d\varrho + \left[\frac{(\bar{r}+1)^2}{3} + \frac{\bar{r}^3}{6}\right], & r \geq \bar{r}+1. \end{cases}$$

Since

$$\widetilde{h}(r) \geq \widetilde{h}(\bar{r}) = h(\bar{r}) = H_0 \quad \text{for } \; r \geq \bar{r},$$

the argument from the beginning of the proof of case (*b*) shows that the extended solution satisfies $|r(t)| \leq \bar{r}$ and, therefore, is a solution of the original problem. □

Remark 1.1 Theorems 1.1–1.3 imply (and are equivalent to) corresponding results on well-posedness of the Cauchy problem for Eq. (1.1) on $\widetilde{l^2} \times l^2$. Certainly, these parallel statements can be obtained directly by similar arguments.

Local Theorem 1.1 applies to all examples considered in Section 1.1 except the singular Lennard-Jones potential. Global existence for the β-model (Example 1.3), as well as for the Toda lattice (Example 1.4), follows immediately from Theorem 1.3. For the α-model (Example 1.2) we expect that global in time solutions do exist for some set of initial data, while for all other initial data the solutions blow up at finite time.

For the lattice with Lennard-Jones potential the existence of global solution holds true for all initial data $u^{(0)} = \left(r^{(0)}, s^{(0)}\right) \in l^2 \times l^2$ such that $r^{(0)}(n) > -d$ for all $n \in \mathbb{Z}$. In this case one can follow the proof of Theorem 1.3, case (*b*), modifying the potential near the singularity and behind it to reduce the problem to a nonsingular one.

1.3 Harmonic lattices

Here we consider *harmonic lattices, i. e.* lattices with quadratic interaction potential

$$U_n(r) = \frac{c(n)}{2}\,r^2.$$

Throughout this section we assume that

(*h*) *there exist positive constants* m_0, M_0 *and* C *such that*

$$0 < m_0 \le m(n) \le M_0$$

and

$$|c(n)| \le C.$$

The dynamics of the harmonic lattice is governed by the equation

$$m\ddot{q} = \partial^+ c\, \partial^- q, \tag{1.20}$$

with the phase space $\widetilde{l^2} \times l^2$ (see Eq. (1.9)). In other words, we consider solutions such that q is a C^1 function with values in $\widetilde{l^2}$, while $\dot{q}$ is a C^1 function with values in l^2.

Making use the change of unknown $x = m^{1/2}q$, we see that Eq. (1.20) is equivalent to the equation

$$\ddot{x} = m^{-1/2}\partial^+ c\, \partial^- m^{-1/2} x \tag{1.21}$$

considered in the phase space $\widetilde{l^2} \times l^2$. Let us introduce the operator A by the formula

$$-Ax = m^{-1/2}\partial^+ c\, \partial^- m^{-1/2} x. \tag{1.22}$$

Notice that the operators $-\partial^+$ and ∂^- are formally adjoint and the same holds true for the operators $-m^{-1/2}\partial^+$ and $\partial^- m^{-1/2}$.

Now Eq. (1.21) becomes

$$\ddot{x} = -Ax. \tag{1.23}$$

The operator A defined by (1.22) is a bounded linear operator in the space $\widetilde{l^2}$ and, actually, the range of A lies in l^2. The last follows from the fact that the operator ∂^- maps $\widetilde{l^2}$ into l^2, while the multiplication by any bounded sequence, as well as the operator ∂^+, leave l^2 invariant. Moreover, being restricted to the space l^2, the operator A is self-adjoint. In what follows the restriction of A to l^2 is still denoted by A.

The Cauchy problem for Eq.(1.20), with

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

is equivalent to the Cauchy problem for Eq. (1.23), with

$$x|_{t=0} = x^{(0)} := m^{1/2}q^{(0)} \in \widetilde{l^2}, \quad \dot{x}|_{t=0} = x^{(1)} := m^{1/2}q^{(1)} \in l^2. \tag{1.24}$$

It is well-known (see, *e. g.*, [Dalec'kii and Krein (1974); Deimling (1977)]) that the solution of (1.23), (1.24) is given by

$$x = \cos\left(tA^{1/2}\right) x^{(0)} + A^{-1/2} \sin\left(tA^{1/2}\right) x^{(1)}, \tag{1.25}$$

where the operator functions $\cos\left(tA^{1/2}\right)$ and $A^{-1/2}\sin\left(tA^{1/2}\right)$ are defined by means of power series expansions

$$\cos\left(tA^{1/2}\right) := \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k}}{(2k)!} A^k,$$
$$A^{-1/2}\sin\left(tA^{1/2}\right) := \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+1)!} A^k.$$

Being considered in the space of all bounded linear operators in $\widetilde{l}^2$, these expansions are norm convergent. The same holds true with $\widetilde{l}^2$ replaced by l^2. Note that in the notations of these functions $A^{1/2}$ has no independent meaning.

Since $x^{(1)} \in l^2$, the function $A^{-1/2}\sin\left(tA^{1/2}\right)$ in the second term on the right hand part of Eq. (1.25) can be considered as a function of *self-adjoint* operator A in l^2. A direct calculation shows that

$$\begin{aligned} \cos\left(tA^{1/2}\right) - I &= \left[\sum_{k=0}^{\infty} \frac{(-1)^{k+1} t^{2k+2}}{(2k+2)!}\right] A \\ &= -\left[\int_0^t A^{-1/2}\sin\left(\tau A^{1/2}\right) d\tau\right] A. \end{aligned}$$

Therefore, formula (1.25) becomes

$$x = x^{(0)} - \left[\int_0^t A^{-1/2}\sin\left(\tau A^{1/2}\right) d\tau\right] Ax^{(0)} + A^{-1/2}\sin\left(tA^{1/2}\right) x^{(1)}. \tag{1.26}$$

Another way to derive (1.26) is to look for the solution of (1.23), (1.24) in the form $x = x^{(0)} + u$, where u is a function with values in l^2, and reduce the problem to the nonhomogeneous Cauchy problem

$$\ddot{u} = -Au - Ax^{(0)}, \quad u|_{t=0} = 0, \quad \dot{u}|_{t=0} = x^{(1)},$$

in the space l^2, with the operator A being self-adjoint.

The advantage of Eq. (1.26) is that, since $x^{(1)}$ and $Ax^{(0)}$ are both in l^2, the solution is expressed in terms of the function $A^{-1/2}\sin\left(tA^{1/2}\right)$ of the *self-adjoint* operator A in l^2.

Actually, A is a second order difference operator of the form

$$(Ax)(n) = a(n)\,x(n+1) + a(n-1)\,x(n-1) + b(n)\,x(n) \tag{1.27}$$

(Jacobi operator), where

$$a(n) = -\frac{c(n)}{\sqrt{m(n)\,m(n+1)}} \tag{1.28}$$

and

$$b(n) = \frac{c(n) + c(n-1)}{m(n)}. \tag{1.29}$$

This follows immediately from Eq. (1.22).

Looking for solutions to Eq. (1.23) in the form[2] $x = \exp(i\omega t)\,u(n)$, we arrive at the spectral problem

$$Au - \lambda u = 0, \tag{1.30}$$

where $\lambda = \omega^2$. The spectral theory of Jacobi operators is well-understood (see, *e. g.*, [Teschl (2000)] and references therein). Since, due to assumption (h), the operator A is a bounded self-adjoint operator in l^2, its spectrum $\sigma(H)$ is a bounded closed subset of $\mathbb{R}$. More precisely, one has (see, *e. g.*, [Teschl (2000)], Lemma 1.8 and (1.151))

Proposition 1.1

(*i*) *Let*

$$a_+ = \sup_{n\in\mathbb{Z}} \Big[b(n) + |a(n)| + |a(n-1)| \Big],$$
$$a_- = \inf_{n\in\mathbb{Z}} \Big[b(n) - |a(n)| - |a(n-1)| \Big].$$

Then $\sigma(A) \subset [a_-, a_+]$.

(*ii*) *If* $c(n) > 0$ *for all* $n \in \mathbb{Z}$, *then the operator* A *is nonnegative,*

$$\sigma(A) \subset \big[0,\ 4\,\|c\|_{l^\infty}\,\|m^{-1}\|_{l^\infty}\big],$$

and 0 is in the essential spectrum $\sigma_{ess}(A)$.

[2] These are standing waves if $\omega \in \mathbb{R}$.

Now let us consider the case of harmonic N-atomic lattices, *i. e.* we assume that $m(n+N) = m(n)$ and $c(n+N) = c(n)$ for all $n \in \mathbb{Z}$. First, we introduce (a discrete version of) the *Floquet transform* as

$$(\mathcal{U}f)(n,\theta) = \sum_{k\in\mathbb{Z}} f(n-kN)\, e^{ix\theta}. \tag{1.31}$$

Sometimes this transform is called *Gelfand transform.* (For the theory of continuous Floquet transform and its applications we refer to [Kuchment (1993)]). The parameter θ is called *quasimomentum.* Observe that

$$(\mathcal{U}f)(n+N,\theta) = e^{i\theta}(\mathcal{U}f)(n,\theta). \tag{1.32}$$

This is the so-called *Floquet condition.* In physics literature this condition is called the *Bloch condition.* Also we have

$$(\mathcal{U}f)(n,\theta+2\pi) = (\mathcal{U}f)(n,\theta), \tag{1.33}$$

i. e. the Floquet transform is 2π-periodic with respect to quasimomentum. Thus, the quasimomentum θ can be considered as the angle coordinate on the unit circle $\mathbb{S}^1$.

The periodicity assumption implies that the operator A commutes with the Floquet transform

$$(\mathcal{U}Af)(n,\theta) = A(\mathcal{U}f)(n,\theta). \tag{1.34}$$

The operator A on the right hand side of Eq. (1.34) acts on the function of the variable n satisfying Floquet condition (1.32), with θ being a parameter.

Let E denote the space of all complex valued functions on the set $I_N = \{0,1,\ldots,N-1\}$ and E_θ the space of all functions u on $\mathbb{Z}$ satisfying the Floquet condition

$$u(n+N) = e^{i\theta}u(n), \quad n \in \mathbb{Z}. \tag{1.35}$$

Being endowed with the standard inner product, E becomes an N-dimensional Euclidian space. The restriction $u|_{I_N}$ defines an isomorphism between E_θ and E. The Floquet transform is a unitary operator

$$\mathcal{U} : l^2 \to L^2(\mathbb{S}^1; E).$$

The inverse operator $\mathcal{U}^{-1}$ is defined by the formula

$$(\mathcal{U}^{-1}v)(n) = \int_{\mathbb{S}^1} v(n,\theta)\frac{d\theta}{2\pi},$$

where $v(n,\theta)$ is extended from I_N to $\mathbb{Z}$ according to (1.35).

The operator A is well-defined on E_θ and is, in fact, a self-adjoint operator. Denote this operator by $A(\theta)$.

What we have described before, can be summarized in terms of direct integrals as

Theorem 1.4 *The Floquet transform provides a unitary equivalence between the operator A and the direct integral expansion*

$$\int_{\mathbb{S}^1}^{\oplus} A(\theta)\frac{d\theta}{2\pi}.$$

For the discussion of the notion of direct integral see, *e. g.*, [Reed and Simon (1978)].

Due to the isomorphism between E_θ and E, the operators $A(\theta)$ can be considered as acting in E. Actually, $A(\theta)$ form a real analytic family of self-adjoint operators in the space E.

Let

$$\lambda_1(\theta) \leq \lambda_2(\theta) \leq \cdots \leq \lambda_N(\theta)$$

be the eigenvalues of $A(\theta)$. The functions $\lambda_j(\theta)$, $j = 1, 2, \ldots, N$, are continuous (actually, piecewise analytic) on $\mathbb{S}^1$. They are called *band functions* or *dispersion relations.* Let

$$\lambda_j^- = \min_{\theta\in\mathbb{S}^1} \lambda_j(\theta), \quad \lambda_j^+ = \max_{\theta\in\mathbb{S}^1} \lambda_j(\theta).$$

Theorem 1.5 *The spectrum $\sigma(A)$ is absolutely continuous and*

$$\sigma(A) = \bigcup_{j=1}^{N} [\lambda_j^-, \lambda_j^+]. \tag{1.36}$$

The intervals in (1.36) are called *spectral bands*, while the intervals $(\lambda_j^+, \lambda_{j+1}^-)$ are called *spectral gaps.* Some of the gaps may be empty (closed). In general, at most $(N-1)$ gaps open up.

The eigenfunctions of $A(\theta)$ are the generalized eigenfunctions of A called *Bloch eigenfunctions.* Corresponding solutions of Eq. (1.23)

$$x(t,n) = \exp(i\omega t)\, u(n), \quad \omega^2 = \lambda_j(\theta),$$

– so-called *Bloch waves* – have infinite energy. If $c \geq 0$, then $A \geq 0$ and $\sigma(A)$ is nonnegative. Therefore, all the eigenfrequencies are real and the Bloch waves are bounded. In the N-atomic case the Bloch waves are proper analoges of plane waves that occur in the monoatomic case.

For more details about spectral theory of periodic Jacobi operators, including generalized eigenfunction expansions, we refer to [Teschl (2000)].

Now we formulate a spectral result on harmonic lattices with impurities. Let $m = \overline{m} + m^{(0)}$ and $c = \overline{c} + c^{(0)}$, where $\overline{m}$ and $\overline{c}$ are N-periodic, while

$$\lim_{|n|\to\infty} m^{(0)}(n) = \lim_{|n|\to\infty} c^{(0)}(n) = 0.$$

Denote by $\overline{A}$ the operator (1.22) with the coefficients $\overline{m}$ and $\overline{c}$.

Theorem 1.6 *$\sigma_{ess}(A) = \sigma(\overline{A})$. If in addition $|n|\, c^{(0)}(n) \in l^1$, then the point spectrum of A is finite and is located in $\mathbb{R} \setminus \sigma(\overline{A})$, and the essential spectrum of A is absolutely continuous.*

See [Teschl (2000)], Theorem 7.11.

Finally, let us consider the case of monoatomic harmonic lattice. The problem reduces to the equation

$$\ddot{x}(n) = c_0^2\big(x(n+1) + x(n-1) - 2x(n)\big), \tag{1.37}$$

where we assume that $c_0 > 0$. The so-called *plane wave* solutions are given by

$$x(t,n) = \exp\big[i(\varkappa n \pm \omega t)\big] = e^{\pm i\omega t} e^{i\varkappa n},$$

where the wavelength $\varkappa^{-1}$ and the frequency ω are related by the dispersion relation

$$\omega = \pm\sqrt{2}\, c_0 \sqrt{1 - \cos\varkappa} = \pm c_0 \sin\frac{\varkappa}{2}.$$

Note that plane waves are just Bloch waves in the monoatomic case.

For the spectral theory of differential and difference operators we refer to [Atkinson (1964); Berezanskii (1968); Berezin and Shubin (1991); Dunford and Schwartz (1988b); Edmunds and Evans (1987); Glazman (1966); Lanczos (1961); Levitan and Sargsyan (1975); Reed and Simon (1978); Schechter (1981)].

1.4 Chains of coupled nonlinear oscillators

Here we consider another lattice model – an infinite *chain of coupled nonlinear oscillators.*

Let $q(n)$ be a generalized coordinate of n-th oscillator and $U_n(r)$ the potential of the oscillator, *i. e.* the dynamics of n-th oscillator is given by

$$\ddot{q}(n) = -U_n'(q(n)),$$

provided the interaction between the oscillators is absent. Suppose that every oscillator interacts with two its neighbors via linear forces. Then the master equations of the system are

$$\ddot{q}(n) = -U_n'(q(n)) + a(n-1)\big(q(n-1) - q(n)\big) - a(n)\big(q(n) - q(n+1)\big), \quad (1.38)$$

where $n \in \mathbb{Z}$.

Let

$$U_n(r) = -\frac{c(n)}{2} r^2 + V_n(r),$$

where $V(0) = V'(0) = 0$. This means that $r = 0$ is a rest point of each oscillator. Set

$$b(n) = c(n) - a(n) - a(n-1).$$

Then Eq. (1.38) becomes

$$\ddot{q}(n) = a(n)\, q(n+1) + a(n-1)\, q(n-1) + b(n)\, q(n) - V_n'(q(n)), \quad n \in \mathbb{Z}. \quad (1.39)$$

We impose the following boundary condition at infinity

$$\lim_{n \to \pm\infty} q(n) = 0. \quad (1.40)$$

This condition means that at infinity the system is at rest.

In what follows we consider the case when the oscillators are anharmonic, *i. e.* $V_n \neq 0$. The case of harmonic chains is described by linear equation (1.23) with $m \equiv 1$ and, hence, reduces to the spectral theory of difference operators.

We impose the following two assumptions (*cf.* assumptions (*i*) and (*ii*) of Section 1.2):

(i') the sequences $a(n)$ and $c(n)$ are bounded;

(ii') the potential $V_n(r)$ is C^1 on $\mathbb{R}$, $V_n(0) = V_n'(0) = 0$ and for every $R > 0$ there exists $C = C(R) > 0$ such that

$$\big|V_n'(r_1) - V_n'(r_2)\big| \leq C|r_1 - r_2|, \quad |r_1 - r_2| \leq R, \quad (1.41)$$

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

The natural configuration space that incorporates boundary condition (1.40) is the space l^2 of two-sided sequences. The corresponding phase space is $l^2 \times l^2$.

Let us introduce the linear operator

$$(Aq)(n) = a(n)\, q(n+1) + a(n-1)\, q(n-1) + b(n)\, q(n)$$

and the nonlinear operator

$$B(q)(n) = -V_n'(q(n)).$$

Under assumptions (i') and (ii') A is a bounded self-adjoint operator in l^2, while the operator B is bounded and locally Lipschitz continuous. Equation (1.39) together with boundary condition (1.40) can be naturally written as an operator differential equation

$$\ddot{q} = Aq + B(q) \tag{1.42}$$

in the space l^2.

Equation (1.42) is a Hamiltonian system on $l^2 \times l^2$, with the Hamiltonian

$$H(q,p) = \frac{1}{2}\left[\|p\|^2 - (Aq,q)\right] + \sum_{n=-\infty}^{+\infty} V_n(q(n)), \tag{1.43}$$

where $p = \dot{q}$. Under assumptions (i') and (ii') $H(p,q)$ is a C^1 functional on $l^2 \times l^2$ and, hence, H is a conserved quantity.

Consider the Cauchy problem for (1.42) with the initial data

$$q|_{t=0} = q^{(0)} \in l^2, \quad \dot{q}|_{t=0} = q^{(1)} \in l^2. \tag{1.44}$$

Its local well-posedness under assumptions (i') and (ii') is a consequence of standard results (*cf.* Theorem 1.1). Exactly as in the case of FPU lattices (see Theorems 1.2 and 1.3) we have also the following results.

Theorem 1.7 *Assume (i') and (ii') with the constant C independent of R. Then for every $q^{(0)} \in l^2$ and $q^{(1)} \in l^2$ Cauchy problem (1.42), (1.43) has a unique solution defined for all $t \in \mathbb{R}$.*

Theorem 1.8 *In addition to assumptions (i') and (ii'), assume that the operator A is non-positive, i. e. $(Aq,q) \le 0$ for all $q \in l^2$. Suppose also that one of the following two conditions holds:*

(a) $V_n(r) \ge 0$ for all $n \in \mathbb{Z}$ and $r \in \mathbb{R}$

or

(b) there exists a nondecreasing function $h(r)$, $r \geq 0$, *such that* $\lim_{r \to +\infty} h(r) = +\infty$ *and* $V_n(r) \geq h(|r|)$ *for all* $n \in \mathbb{Z}$ *and* $r \in \mathbb{R}$.

Then for every $q^{(0)} \in l^2$ *and* $q^{(1)} \in l^2$ *problem (1.42), (1.43) has a unique solution defined for all* $t \in \mathbb{R}$.

As it follows from the next proposition, under some additional condition one can skip the assumption of nonpositivity of A in Theorem 1.8.

Proposition 1.2 *Under assumptions of Theorem 1.8, case (b), without* $(Aq, q) \leq 0$, *suppose that*

$$\lim_{r \to +\infty} \frac{h(r)}{r^2} = +\infty.$$

Then problem (1.42), (1.43) has a unique global solution for every $q^{(0)} \in l^2$ *and* $q^{(1)} \in l^2$.

Proof. Write the potential U_n in the form

$$U_n(r) = -\frac{c(n) - 2\lambda}{2} r^2 + \left(V_n(r) - \lambda r^2\right),$$

with $\lambda > 0$ large enough. Then the new operator A that corresponds to the coefficients $a(n)$ and $c(n) - 2\lambda$ is non-positive. At the same time

$$V_n(r) - \lambda r^2 \geq h(|r|) - \lambda r^2 = h(|r|) \left(1 - \lambda \frac{r^2}{h(|r|)}\right).$$

This yields

$$V_n(r) - \lambda r^2 \geq k_1 h(|r|) - k_2,$$

with some $k_1 \in (0, 1)$ and $k_2 \geq 0$. Now it is enough to apply Theorem 1.8, with $h(r)$ replaced by $k_1 h(r) - k_2$. The proof is complete. □

Now we consider few examples. In all these examples $a(n)$ and $U_n(r)$ do not depend on $n \in \mathbb{Z}$.

Example 1.6 Taking $a(n) \equiv a > 0$, $c(n) \equiv 0$ and

$$V_n(r) = 1 - \cos r,$$

one obtains the *Frenkel-Kontorova model*. The master equation of this model reads

$$\ddot{q}(n) = a\,(\Delta_d q)(n) - \sin q(n), \tag{1.45}$$

where

$$(\Delta_d q)(n) = q(n+1) + q(n-1) - 2q(n)$$

is the 1-dimensional discrete Laplacian. Equation (1.45) is a straightforward discretization of the famous sin-Gordon equation

$$q_{tt} - a q_{xx} + \sin q = 0.$$

The last equation is a completely integrable system (see, *e. g.* [Ablowitz and Segur (1981)]). At the same time its discrete counterpart, Eq. (1.45), is *not* completely integrable.

Example 1.7 When $a(n) \equiv a > 0$, $c(n) \equiv -m^2 \le 0$ and

$$V_n(r) = -\frac{\lambda}{k+1}\, r^{k+1}, \quad k > 0 \text{ integer},$$

we obtain the *discrete nonlinear Klein-Gordon (DNKG) equation* ($m^2 > 0$)

$$\ddot{q}(n) = a\,(\Delta_d q)(n) - m^2 q(n) + \lambda q^k(n) \tag{1.46}$$

and *discrete nonlinear wave (DNW) equation* ($m^2 = 0$)

$$\ddot{q}(n) = a\,(\Delta_d)(n) + \lambda q^k(n). \tag{1.47}$$

The cubic ($k = 3$) and quadratic ($k = 2$) cases are of particular interest.

Example 1.8 If $a(n) \equiv a > 0$, $c(n) \equiv -m^2 \le 0$ and

$$V_n(r) = -\frac{\lambda}{p+1}\, |r|^{p+1}, \quad p > 0,$$

we obtain the modified discrete Klein-Gordon ($m^2 > 0$) and nonlinear wave ($m^2 = 0$) equations

$$\ddot{q} = a\,\Delta_d q - m^2 q + \lambda |q|^{p-1} q$$

and

$$\ddot{q} = a\,\Delta_d q + \lambda |q|^{p-1} q,$$

respectively.

Example 1.9 If $a(n) \equiv a$, $c(n) = m^2 > 0$ and

$$V_n(r) = \frac{\lambda}{4} r^4, \quad \lambda > 0,$$

then we obtain the so-called *discrete φ^4-equation*

$$\ddot{q} = a\Delta_d q + m^2 q - \lambda q^3 = 0. \tag{1.48}$$

If $\lambda > 0$ and k is odd, then it follows from Theorem 1.8 that the Cauchy problem for equaions from Example 1.7 is globally well-posed. The same holds in Example 1.8 with $\lambda > 0$ and $p > 1$. This is so, because in those cases the operator

$$A = a\,\Delta_d - m^2$$

is a non-positive operator defined in l^2. The Cauchy problem for the quadratic DNKG equation with any $\lambda \neq 0$ has a unique global solution for *small initial data*, as it follows from Theorem 1.9 below.

Let

$$V_n(r) = -\frac{\lambda(n)}{3} r^3,$$

where $\lambda(n)$ is a bounded sequence. Also we suppose that the operator A is negative definite, *i. e.* there exists $\alpha_0 > 0$ such that

$$(Aq, q) \leq -\alpha_0 \|q\|_{l^2}^2 \quad \forall q \in l^2.$$

Set

$$\varphi(q) = -\frac{1}{2}\,(Aq, q) - \frac{1}{3} \sum_{n\in\mathbb{Z}} \lambda(n)\, q^3(n) =: \frac{1}{2}\,\varphi_0(q) + \frac{1}{3}\,\varphi_1(q).$$

Note that $\varphi_0(q)^{1/2}$ is an equivalent norm on l^2. We have that

$$H(p, q) = \frac{1}{2}\,\|p\|_{l^2}^2 + \varphi(q).$$

Since

$$\left|\varphi_1(q)\right| \leq c' \|q\|_{l^3}^3 \leq c'' \|q\|_{l^2}^3,$$

there exists a constant $\kappa > 0$ such that

$$\left|\varphi_1(q)\right|^{1/3} \leq \kappa\, \varphi_0(q)^{1/2}, \quad q \in l^2. \tag{1.49}$$

Let

$$\gamma := \inf \left\{ \sup_{\tau \geq 0} \varphi(\tau q) \ : \ q \in l^2, q \neq 0 \right\}. \tag{1.50}$$

We have that

$$\gamma \geq \frac{1}{6\kappa^6}. \tag{1.51}$$

Indeed,

$$\varphi(\tau q) = \frac{\tau^2}{2}\, \varphi_0(q) + \frac{\tau^3}{3}\, \varphi_1(q).$$

If $\varphi_1(q) \geq 0$, then

$$\sup_{\tau \geq 0} \varphi(\tau q) = +\infty.$$

If $\varphi_1(q) < 0$, then, maximizing the cubic polynomial $\varphi(\tau q)$, we obtain that

$$\sup_{\tau \geq 0} \varphi(\tau q) = \varphi\left(-\frac{\varphi_0(q)}{\varphi_1(q)}\, q \right) = \frac{1}{6}\, \frac{\varphi_0(q)^3}{\varphi_1(q)^2},$$

and the required follows from (1.49).

Now let us define

$$W = \left\{ q \in l^2 \ : \ 0 \leq \varphi(\tau q) < \gamma \quad \forall \tau \in [0,1] \right\}.$$

It is readily verified that the set W is star-shaped with respect to the origin, *i. e.* if $q \in W$, then $\theta q \in W$ for every $\theta \in [0, 1]$.

Lemma 1.2 *For every $\varrho > 0$ such that*

$$\varrho \leq \frac{9}{4\kappa}, \quad \frac{\varrho}{2} + \frac{\kappa^2}{3}\, \varrho^{3/2} < \gamma,$$

the set W contains the open set

$$B = \left\{ q \in l^2 \ : \ \varphi_0(q) < \varrho \right\}.$$

Proof. By (1.49),

$$\frac{\tau^2}{2}\, \varphi_0(q) - \frac{\tau^3\kappa^3}{3}\, \varphi_0(q)^{3/2} \leq \varphi(\tau q) \leq \frac{\tau^2}{2}\, \varphi_0(q) + \frac{\tau^3\kappa^3}{3}\, \varphi_0(q)^{3/2}.$$

Thus, $\varphi(\tau q) \geq 0$ for every $\tau \in [0, 1]$, provided

$$\frac{1}{2} - \frac{\tau\kappa^3}{3}\, \varphi_0(q)^{1/2} \geq 0 \quad \forall \tau \in [0,1].$$

Hence, if $\varphi_0(q) \leq 9/(4\kappa^2)$, the second condition for ϱ implies that $\varphi(\tau q) < \gamma$. $\square$

Let

$$W_* = \left\{q \in l^2 \ : \ \varphi_0(q) + \varphi_1(q) > 0, \ \varphi(q) < \gamma\right\}.$$

By the continuity of the functionals φ_0, φ_1 and φ, the set W_* is open.

Lemma 1.3 *We have that $W = W_* \cup B$.*

Proof. Due to Lemma 1.2, it sufficies to show that $W = W_* \cup \{0\}$.

Let $q \in W$, $q \neq 0$. If $\varphi_1(q) \geq 0$, then $\varphi_0(q) + \varphi_1(q) > 0$ and obviously $\varphi(q) < \gamma$.

If $\varphi_1(q) < 0$, then

$$\sup_{\tau \geq 0} \varphi(\tau q) = \varphi\left(-\frac{\varphi_0(q)}{\varphi_1(q)}\, q\right) \geq \gamma.$$

Hence, $-\varphi_0(q)/\varphi_1(q) > 1$ and $\varphi(q) < \gamma$. This implies that $q \in W_*$.

Conversely, let $q \in W_*$. If $\varphi_1(q) \geq 0$, then

$$\sup_{\tau \in [0,1]} \varphi(\tau q) = \varphi(q) < \gamma$$

and $q \in W$.

If $\varphi_1(q) < 0$, then the inequality $-\varphi_0(q)/\varphi_1(q) > 1$ implies that

$$\sup_{\tau \in [0,1]} \varphi(\tau q) = \varphi(q)$$

and we conclude. $\square$

Since W_* and B are open set, the set W is open.

Lemma 1.4 *The set W is bounded.*

Proof. If $\varphi_1(q) \geq 0$, then $\varphi(q) \geq \varphi_0(q)/2$ and $\varphi_0(q) > 2\gamma$.

If $\varphi_1(q) < 0$, then Lemma 1.3 shows that $\varphi_1(q) > -\varphi_0(q)$. Hence, $\varphi(q) > \varphi_0(q)/6$ and $\varphi_0(q) < 6\gamma$. Thus, $W \subset \{q \in l^2 \ : \ \varphi_0(q) < 6\gamma\}$, *i. e.* W is contained in a bonded set and we conclude. $\square$

Now we are ready to prove

Theorem 1.9 *Suppose that the operator A is negative definite and*

$$V_n(r) = -\frac{\lambda(n)}{3}\, r^4,$$

where the sequence $\lambda(n)$ is bounded. Let $q^{(0)} \in W$ and $q^{(1)} \in l^2$ satisfy

$$\frac{1}{2}\left\|q^{(1)}\right\|_{l^2}^2 + \varphi\left(q^{(0)}\right) < \gamma.$$

Then the Cauchy problem for (1.42) with the initial data $q^{(0)}$ and $q^{(1)}$ has a unique global solution.

Proof. The existence and uniqueness of the local solution $q(t)$ is obvious. To prove that $q(t)$ extends to a solution defined for all $t \in \mathbb{R}$ it is enough to show that $q(t)$ remains bounded.

We show that $q(t) \in W$. Assume not. Let $t_1 > 0$ be the smallest value of $t > 0$ for which $q(t) \notin W$. Then $q(t_1) \in \partial W$, the boundary of W. Since W is a star-shaped set, then $\theta q(t_1) \in W$ for all $\theta \in [0, 1]$. Hence, $\varphi(\theta q(t_1)) < \gamma$. Passing to the limit as $\theta \to 1$, we obtain that $\varphi(q(t_1)) \leq \gamma$.

If $\varphi(q(t_1)) < \gamma$, then, by definition of W and the fact that $\varphi(\theta\, q(t_1)) < \gamma$ $\forall \theta \in [0, 1)$, we conclude that $q(t_1) \in W$, a contradiction. Hence

$$\varphi(q(t_1)) = \gamma.$$

Since the Hamiltonian H is a conserved quantity, we have that

$$\begin{aligned}\gamma = \varphi(q(t_1)) &\leq H(p(t_1), q_1(t_1)) = \frac{1}{2}\left\|\dot{q}(t_1)\right\|_{l^2}^2 + \varphi(q(t_1)) \\ &= H\left(q^{(0)}, q^{(1)}\right) = \frac{1}{2}\left\|q^{(1)}\right\|_{l^2}^2 + \varphi\left(q^{(0)}\right) \\ &< \gamma.\end{aligned}$$

This contradiction shows that $q(t) \in W$ and, hence, $q(t)$ remains bounded for all $t > 0$.

Since Eq. (1.42) is invariant with respect to the inversion of time, the same holds for $t < 0$ and the proof is complete. $\square$

Note that the assumptions on $q^{(0)}$ and $q^{(1)}$ are satisfied when the norms $\|q^{(0)}\|$ and $\|q^{(1)}\|$ are small enough.

1.5 Comments and open problems

In Sections 1.1–1.2 we have presented, in an appropriate form, more or less commonly known results. Theorem 1.3 is an extension of the global existence result given in [Friesecke and Pego (1999)].

For many nonlinear wave type equations global solution do exist for *small*, in an appropriate sense, initial data (see, *e. g.*, [Reed and Simon (1979); Reed (1976)]). The following problem remains open.

Problem 1.1 *Is it possible to find a norm in the phase space so that smallness of initial data would imply global existence for the* α*-model?*

The study of FPU lattices was initiated by E. Fermi, J. Pasta and S. Ulam in [Fermi *et. al* (1955)]. Since that time it is appeared an extensive physics literature on FPU type chains, as well as articles devoted to numerical simulation of lattice systems. See [Braun and Kivshar (1998); Braun and Kivshar (2004); Eilbeck (1991); Eilbeck and Flesch (1990); Flach and Willis (1998); Flytzanis *et. al* (1989); Peyrard *et. al* (1986); Rosenau (1989); Wattis (1993a); Wattis (1993b); Wattis (1996)], to mention a few. Applications of the Frenkel-Kontorova model in physics are discussed in [Braun and Kivshar (1998); Braun and Kivshar (2004)].

The contents of Section 1.4 is borrowed from [Bak and Pankov (to appear)]. In fact, Theorem 1.9 is a discrete counterpart of a result on nonlinear hyperbolic equations obtained in [Sattinger (1968)] (see also [Lions (1969)]).

We point out the following problems.

Problem 1.2 *Investigate global well-posedness of the Cauchy problem for DNKG and DNW equations in the case when* $\lambda < 0$ *and* k *is odd.*

Problem 1.3 *Study global well-posedness of Cauchy problem for the discrete* φ^4*-equation.*

Since DNKG and DNW equations are discrete counterparts of continuum KG and wave equations, it is natural to study the following

Problem 1.4 *When DNKG and DNW equations possess nonlinear scattering?*

Basic facts on nonlinear scattering theory (for classical continuum wave equations) can be found in [Reed (1976); Reed and Simon (1979)] and [Strauss (1989)].