Atomistic to Continuum Models for Crystals

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To my parents

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Abstract

The theory of nonlinear mass-spring chains has a history stretching back to the now famous numerical simulations of Fermi, Pasta and Ulam. The unexpected results of that experiment have led to many new fields of study. Despite this, the mathematics of the lattice equations have proved sufficiently rich to attract continued attention to the present day.

This work is concerned with the motions of an infinite one dimensional lattice with nearest-neighbour interactions governed by a generic potential. The Hamiltonian of such a system may be written

$$H = \sum_{i=-\infty}^{\infty} \left(\frac{1}{2} p_i^2 + V(q_{i+1} - q_i) \right),$$

in terms of the momenta p_i and the displacements q_i of the lattice sites. All sites are assumed to be of equal mass. Certain generic conditions are placed on the potential V.

Of particular interest are the solitary wave solutions which are known to exist upon such lattices. The KdV equation has long been known to emerge in a formal manner from the lattice equations as a continuum limit. More recently, the lattice's localized nonlinear modes have been rigorously approximated by the KdV's well-studied soliton solution, in the lattice's long wavelength regime. To date, however, little is known about how, and to what extent, lattice solitary waves *differ* from KdV solitons.

It is proved in this work that a solution (which we prove to be unique) to a particular linear ordinary differential equation provides a correction to the KdV approximation. This gives, in an explicit way, the lowest order effect of lattice discreteness upon lattice solitary waves.

It is also shown how such discreteness effects are propagated along the lattice both in isolation (single soliton case), and in the presence of another soliton correction (the bisoliton case). In the latter case their interaction is studied and the impact of lattice discreteness upon lattice solitary wave interactions is observed. This is possible by virtue of the discovery of an evolution equation for discreteness effects on the lattice. This equation is proved to have appropriate unique solutions and is found to be strikingly similar to corresponding equations known in both the theories of shallow water waves and ion-acoustic waves.

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Chapter 1

Background and Context

1.1 The historical background

Among the first pioneers in the subject of one-dimensional mass-spring chain oscillations were three people whose names have become famously linked to it: Enrico Fermi, John Pasta and Stanislaw Ulam (FPU). By the 1950s it was known that a chain of masses linked by springs with linear restoring forces would continue to oscillate indefinitely in the energy mode(s) of the initial condition (see Subsection 1.5.1). FPU's well-known 1955 numerical experiment [FPU55] was designed to discover the extent to which inclusion of a nonlinearity in the restoring force would cause excitation of modes not initially activated. It was conjectured that energy would eventually 'thermalize', i.e. become equidistributed among all possible modes. However, the experiment revealed instead that energy ran through successive modes, exciting one mode only as the energy in another diminished. This behaviour persisted so that after a certain time the initial conditions were revisited - a phenomenon dubbed 'recurrence'. This process was observed to continue indefinitely with almost complete periodicity and virtually no thermalization.

Two possible explanations might be put forward for the existence of such recurrences: they may either be linear recurrences (the recurrences which would be expected in the linearized system) or they might be the recurrences predicted to exist by Poincaré's Recurrence Theorem for a volume preserving one-to-one map on a bounded region of Euclidean space into itself. However, examination of the period of the recurrence discounts either of these possibilities: linear recurrences have a period 50 times smaller than FPU recurrences, whereas Poincaré recurrences are estimated to have a period of the order of 10^{33} times larger [TM72].

The so-called (periodic) 'FPU' chain which was used in their experiment consisted of 64 unit masses linked together by identical springs whose restoring force was *non-*

linear. The springs' potential (known later as the FPU potential) could be written as $(1/2)\alpha r^2 + (1/3!)\beta r^3$ for constants $\alpha > 0$ and $\beta \neq 0$ and for a displacement r from equilibrium spacing.

An adequate explanation for the FPU's observations was not found until 1965 when Zabusky and Kruskal [ZK65] were able to derive the already well-known Korteweg-de Vries (KdV) equation from the FPU lattice equations (given explicitly below) by taking a formal continuum limit. They then simulated the KdV equation with periodic boundary conditions numerically and found that despite the equation's nonlinearity, initial conditions eventually decomposed into coherent parts travelling with different wave speeds and, most remarkably of all, interacting extremely 'cleanly', in a manner reminiscent of linear superposition. The only lasting indication that a nonlinear interaction had taken place at all was a phase shift. The coherent parts of the solution were named 'solitons' and their unusual stability during interaction, it was suggested, lay at the root of the FPU recurrences. Energy could be transported along the lattice indefinitely without dispersion due to the existence and resilience of solitons.

Zabusky and Kruskal's derivation of the KdV equation from the lattice equation, although not rigorous, is historically significant enough to justify its reproduction: take $q_i = q_i(t)$ to denote the displacement of the i^{th} lattice site from equilibrium at time t (so that $r(= r_i) = q_{i+1} - q_i$ may be considered to be the *relative* displacement from equilibrium). Throughout this work we shall assume that the sequence r (as well as the sequence $p := \partial_t r$ corresponding to lattice momenta) belongs to the finite energy space l^2. We do not impose boundary conditions during the derivation: zero boundary conditions will lead to a zero boundary condition KdV problem,[1] whereas periodic boundary conditions will lead to a periodic KdV problem.

If the masses are normalised and the restoring force is given by $\alpha(q_{i+1} - q_i) + 1/2\beta(q_{i+1} - q_i)^2$, the equations which govern the dynamics of the lattice with FPU potential are

$$\partial_{tt} q_i = \left[\alpha(q_{i+1} - q_i) + 1/2\beta(q_{i+1} - q_i)^2\right] - \left[\alpha(q_i - q_{i-1}) + 1/2\beta(q_i - q_{i-1})^2\right]. \quad (1.1)$$

[1] Throughout this work, when dealing with *infinite* lattices, we use the terminology 'zero boundary condition' to mean $r_i \to 0$ as $i \to \pm\infty$. Note that we therefore only impose boundary conditions on the *difference* $q_{i+1} - q_i$ and not upon q_i itself. The implication is that it is acceptable for a lattice site close to $\pm\infty$ to be "displaced from equilibrium" (although for definiteness we shall see that it is natural to take $q_i \to 0$ as $i \to -\infty$) as long as the *relative* displacement is zero. On the other hand, in keeping with standard practice, we will, in Subsection 1.5.1 when dealing with the *finite* dimensional lattice, use $q_0 = q_{N+1} = 0$ to denote the 'clamping' of the boundary sites.

By some rearrangement this leads to

$$\partial_{tt} q_i = \alpha(q_{i+1} - 2q_i + q_{i-1})\Big[1 + \frac{1}{2}\frac{\beta}{\alpha}(q_{i+1} - q_{i-1})\Big]$$

and thence, by Taylor expanding q_{i+1} and q_{i-1} in terms of q_i with spring length denoted by h, to

$$\partial_{tt} q = \alpha h^2 \Big(\partial_{xx} q + \frac{h^2}{12}\,\partial_{xxxx} q\Big)\Big(1 + \frac{\beta}{\alpha}\,h\,\partial_x q\Big)\,,$$

dropping the i subscript.[2] Set $\alpha h^2 =: c^2$, $h\beta/\alpha =: \varepsilon$ and $h^2/12\varepsilon =: \delta^2$. Here ε and h are treated as small parameters, although δ^2 is *not* (this may seem somewhat arbitrary, but is necessary if the second approximation to the finite difference $q_{i+1} - 2q_i + q_{i-1}$ is to be included in the final approximating equation). The equation then becomes (dropping products of two 'small' terms)

$$\partial_{tt} q - c^2 \partial_{xx} q = \varepsilon c^2 \partial_x q \partial_{xx} q + \varepsilon c^2 \delta^2 \partial_{xxxx} q\,.$$

We look for solutions which are approximately travelling waves with at most 'slowly' varying form and so we set

$$q = q^{(0)}(\xi, T) + \varepsilon q^{(1)}(x, t) + \cdots\,,$$

where $\xi := x - ct$ and $T := \varepsilon t$. Note that c is taken as the wavespeed by analogy with the parameter c in the wave equation

$$\partial_{tt} q = c^2 \partial_{xx} q\,.$$

At order ε we recover the following equation:

$$2cq^{(0)}_{\xi T} + c^2 q^{(0)}_{\xi} q^{(0)}_{\xi\xi} + c^2\delta^2 q^{(0)}_{\xi\xi\xi\xi} = 0\,.$$

Writing $u := q^{(0)}_{\xi}$ and $\tau := cT/2$, this becomes

$$u_\tau + u u_\xi + \delta^2 u_{\xi\xi\xi} = 0\,,$$

which is the KdV equation.

For many researchers, the most interesting aspect of Zabusky and Kruskal's work was the clean interactions between the KdV solitons which they discovered. This

[2] The key insight of [ZK65] in respect of this formal derivation was to drop terms smaller than $\mathcal{O}(h^2)$ contained in the second bracket on the right-hand-side, but to keep terms up to $\mathcal{O}(h^4)$ in the first bracket. This ensures that a dissipative term appears in the final approximation.

unexpected phenomenon led to a large outpouring of work on the KdV equation and other equations displaying similar behaviour such as the nonlinear Schrödinger equation. The body of knowledge thus acquired is now known as the theory of Inverse Scattering and completely integrable systems ([GGKM67], [Lax68], [ZS72], [AKNS74], [ZS74]), [CD82], [Zak98]). In particular, the theory has led to proofs for the existence of *multi*-soliton solutions for KdV and to closed-form expressions for them [GGKM67].

Although the behaviour of soliton solutions to the KdV equation is now well-understood, the link between the FPU lattice equations and KdV has remained, until recently, formal. Moreover, despite a substantial body of physics literature on discrete lattice systems, little *mathematical* attention has been paid to the difference in form and behaviour between KdV soliton solutions and the corresponding lattice solitary waves.

1.2 Hamiltonian context of the lattice problem

The FPU lattice equations arise as the equations of motion for the Hamiltonian

$$H = \sum_{i=-\infty}^{\infty} \left(\frac{1}{2} p_i^2 + V(q_{i+1} - q_i) \right),$$

where $q_i = q_i(t)$ and $p_i = p_i(t)$ denote the displacement and momentum of the i^{th} lattice site at time t and V is the potential of the springs (all identical). For example, as indicated above, the FPU potential is $V(r) = (1/2)\alpha r^2 + (1/3!)\beta r^3$, where r denotes the distortion of a lattice spring from its equilibrium length, so that at the i^{th} lattice site $r(i,t) =: r_i = q_{i+1} - q_i$. Using the notations $\partial_{tt} r = \ddot{r} = \partial_t^2 r$ interchangeably throughout this work to denote the second derivative of r with respect to time, the generic equations of motion read

$$\partial_t^2 r = (e^{\partial} - 2 + e^{-\partial}) V'(r) \tag{1.2}$$

- cf. (1.1) above - where e^{∂} and $e^{-\partial}$ denote (respectively) the forward and backward shifts along the lattice:

$$e^{\partial} r(t,i) = r(t,i+1), \qquad e^{-\partial} r(t,i) = r(t,i-1)\,.$$

Before continuing, we point out that our problem is stated, in essence, in terms of q_i (for example, p_i is defined in terms of $\dot{q}_i$). Our intention throughout the remainder of this work, however, is to treat r_i (rather than q_i) as the important dependent

variable. This is not a major difference because the equations of motion are given solely in terms of r_i and because we have the relation

$$q_i = \sum_{j=-\infty}^{i-1} r_j \,. \tag{1.3}$$

This relation implies, in particular, that $q_i \to 0$ as $i \to -\infty$, which amounts to stipulating that the leftmost part of the disturbed lattice is aligned with an undisturbed lattice, relative to which the q_i are measured. Although it is conceivable that, for certain motions of the lattice, the right-hand-side of (1.3) does not converge, for the purposes of this work we are able to guarantee convergence by virtue of part (c) of Theorem 1.1 in [FP99] which states that the lattice solitary wave solution r_j falls off exponentially as $j \to \pm\infty$. It now makes sense for us to use r_i as our underlying variable. q_i may then be retrieved from r_i as indicated.

Now, note that (1.2) may be written as a system of two first order equations as follows:

$$\partial_t u = JDH(u) \tag{1.4}$$

where

$$u := \begin{pmatrix} r \\ p \end{pmatrix}, \qquad J := \begin{pmatrix} 0 & e^{\partial} - 1 \\ 1 - e^{-\partial} & 0 \end{pmatrix}$$

and $DH(u) = (V'(r), p)$ is the functional gradient of H. If the inner product

$$\langle u, \tilde{u} \rangle = \left\langle \begin{pmatrix} r \\ p \end{pmatrix}, \begin{pmatrix} \tilde{r} \\ \tilde{p} \end{pmatrix} \right\rangle := \sum_{j=-\infty}^{\infty} \big(r(j)\tilde{r}(j) + p(j)\tilde{p}(j) \big)$$

on $l^2(\mathbb{Z})$ is used, (1.4) is consistent with the general 'Hamiltonian form', defined to be

$$u_t = J \frac{\partial H}{\partial u} \,, \tag{1.5}$$

where J is a linear skew operator ($J^* = -J$). We therefore call the system Hamiltonian and note that it has a countable infinity of degrees of freedom. Systems of this size (although considerably larger than the 64 particle system considered by FPU) are of current interest due to the fact that large systems are much more likely to display behaviour encountered in physical situations.

Generally speaking, Hamiltonian systems with, say, $2N$ degrees of freedom, will conserve a certain number of quantities for all time. These are the constants of the motion, and energy (given by the Hamiltonian itself) is an example. Each constant of the motion constrains the flow of the solution in $2N$-dimensional phase space. In some (exceptional) circumstances, a Hamiltonian system will possess as many constants of

the motion as it has position co-ordinates (i.e. N). In this situation, the system is called 'integrable' and the motion is constrained to lie on the N-dimensional surfaces of tori in $2N$-dimensional phase space. The reason for the name 'integrable' stems from Liouville's Theorem in classical mechanics (e.g. [Arn89], p.272) which states that if N 'first integrals' (i.e. conserved quantities) are known and are 'in involution' (i.e. there exists a Poisson bracket[3] such that the Poisson bracket of each pair of conserved quantities is identically zero), then the $2N$ canonical equations of the Hamiltonian system may be integrated - i.e. each first integral reduces the order of the canonical equations by not just one, but two.

Another important aspect of integrable systems is that it is possible to transform the original position and momentum coordinates into a canonical set of symplectic coordinates[4] known as the 'action-angle' coordinates $(\mathbf{I}, \theta)$. In these coordinates the equations of motion for the Hamiltonian H take the simple form

$$\frac{\mathrm{d}\mathbf{I}}{\mathrm{d}t} = \mathbf{0}\,, \qquad \frac{\mathrm{d}\theta}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{I}}\,.$$

Hence, the coordinates $\mathbf{I}$ represent constants of the motion and, in fact, any conserved quantity may be expressed in terms of them. In particular, $H = H(\mathbf{I})$.

Although integrable systems are known to be non-generic, some of the so-called 'invariant' tori present in such systems (ones where the motions around the tori are 'incommensurate') are known to persist (in approximate form) even when non-integrable perturbations are applied to the Hamiltonian. This is the essence of a Theorem by Kolmogorov, Arnold and Moser (KAM) (e.g. [Arn89]). It implies that an integrable system is capable of imposing structure upon the phase space flow of a"near-by" non-integrable system. However, the extent of this imposition is dependent upon the fraction of phase space which the invariant tori occupy, and this depends upon the number of degrees of freedom - i.e. upon N. Hamiltonian systems with large N and where the interaction between particles within the system is only *short range* (i.e. the interaction between particles decays rapidly with increasing separation) have been studied by Wayne [Way84]. It was found that the fraction of phase space covered by

[3]A Poisson bracket of two functions F and G on a smooth manifold M is defined to be a skew-symmetric bilinear map $(\cdot,\cdot) : C^\infty(M) \times C^\infty(M) \to C^\infty(M)$ which satisfies the 'Leibniz rule' $(FG, H) = F(G, H) + G(F, H)$ and the 'Jacobi identity' $(F, (G, H)) + (G, (H, F)) + (H, (F, G)) = 0$. Within this context, a Hamiltonian is a function $H \in C^\infty(M)$ satisfying $\mathrm{d}/\mathrm{d}t|_{t=0} F(g^t(x)) = (F, H)(x)$, for some given phase flow $g^t : M \to M$.

[4]A set of coordinates $(\mathbf{p}, \mathbf{q})$ is called 'symplectic' (with respect to a given symplectic manifold) if the symplectic form ω^2 of the manifold is expressible as $\omega^2 = \mathrm{d}p_1 \wedge \mathrm{d}q_1 + \cdots + \mathrm{d}p_N \wedge \mathrm{d}q_N$.

invariant KAM tori decreases with N. In particular, the fraction decreases no faster than proportional to N^{-160} as $N \to \infty$[5], although more recently, Pöschel [Pos90], has succeeded in showing that the rate is, in fact, closer to N^{-48}.

Wayne and Pöschel's results are important in the context of FPU chains because physical springs (for example those modelling interatomic forces), give rise to only short-range interactions between particles in the system. Moreover, unless very specific (non-generic) potentials are used (see Subsection 1.5.2), the lattice equations will be non-integrable and so (assuming they are not *too* far from being integrable) a KAM approach to solving them may be appropriate. Indeed, in small sized systems (such as the 64 particles studied by FPU) such an approach is successful (for example, [Rin00], [Rin01]). However, for infinite dimensional systems even Wayne and Pöschel's upper bounds on the rate of decrease of phase space covering are not sufficient to avoid the conclusion that a perturbation theory approach is unlikely to succeed.

1.3 Hamiltonian structure of the KdV equation

Another approach to solving the FPU lattice equations might be made by exploiting their "closeness" to the KdV equation. This again involves the theory of Hamiltonian systems because, as discovered by Gardner [Gar71], the KdV equation has itself the natural structure of an infinite dimensional integrable Hamiltonian system. Indeed, the KdV equation

$$u_t = -u_{xxx} + 6uu_x$$

may be written in Hamiltonian form

$$\frac{\partial u}{\partial t} = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial H}{\partial u}\,,$$

where

$$H(u) = \int \left(\frac{1}{2}u_x^2 + u^3\right) \mathrm{d}x$$

and where $\partial H/\partial u$ denotes the Fréchet derivative of H with respect to the standard scalar product on $L^2(\mathbb{R})$.[6] Indeed this is consistent with the general Hamiltonian form given in (1.5).

[5]This result makes considerable use of the fact that the interactions are short range. Without this assumption the best estimate for the fraction is around $(N!)^{-31}$ as $N \to \infty$.

[6]At this point it is worth noting the notational distinction between Hamiltonians - written with a simple H - and the Sobolev spaces $H^N(A)$ of functions with domain A, which will always display a numeric superscript.

Following Arnold ([Arn89], p.454), a symplectic structure ω^2 may be defined upon the Sobolev space $H^N(\mathbb{R}) =: M$ (for any $N \geq 1$) by the formula

$$\omega^2_{[u]} := \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{x} \mathrm{d}y \big(\mathrm{d}u(x) \wedge \mathrm{d}u(y)\big) \,.$$

The phase flow $g^t_H : M \to M$, corresponding to the Hamiltonian H, with parameter $t \in \mathbb{R}$ preserves this structure:

$$(g^t_H)^* \omega^2 = \omega^2 \,,$$

where $(g^t_H)^*$ is defined in terms of the differential $\mathrm{d}g^t_H$ of g^t_H by the formula:

$$(g^t_H)^* \omega^2(\xi_1, \xi_2) = \omega^2\big(\mathrm{d}g^t_H(\xi_1), \mathrm{d}g^t_H(\xi_2)\big) \,,$$

for any pair ξ_1, ξ_2 in the tangent space TM_x of M at some $x \in M$.

Moreover, Gardner [Gar71] also showed that the space of differentiable *spatially periodic* functions, to which the solutions of the periodic boundary condition problem belong, denoted by $H^N(S^1) =: M_{\mathrm{PER}}$ where $S^1 := \mathbb{R}/\mathbb{Z}$, can be endowed with a bracket

$$(F, G) = \int_{S^1} \frac{\partial F}{\partial u} \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial G}{\partial u} \, \mathrm{d}x \,,$$

for functionals F and G on M_{PER} and where $\partial/\partial u$ denotes the L^2 Fréchet derivative. It may be shown that, on M_{PER}, this bracket possesses the Leibniz and Jacobi properties, thus making it a Poisson bracket, as defined on page 6. This makes M_{PER} into a Poisson manifold on which the KdV equation may be represented in the form

$$u_t = \big(u, H\big) \,,$$

where H is the KdV Hamiltonian, as before. This is then reminiscent of the general Poisson form

$$\dot{F} = (F, G) \,,$$

in which $\dot{F}$ is interpreted with respect to the phase flow g^t_G of the Hamiltonian G:

$$\dot{F} := \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} F(g^t_G) \,.$$

Hence, the Hamiltonian structure of the KdV equation has been well studied. A major achievement of this approach was an understanding of the integrable nature of KdV, as set out by Zakharov and Faddeev [ZF71]. Their work demonstrated that the process of 'Scattering' and 'Inverse Scattering' developed by Gardner *et al* [GGKM67] for the purpose of solving the KdV equation exactly was very closely related to the

transformation into and out of the canonical action-angle variables of an integrable system.[7]

The process of Inverse Scattering proceeds by treating the initial condition $u(x)$ for the KdV equation as a potential for the Schrödinger eigenvalue problem

$$-\psi_{xx} + u(x)\psi = k^2\psi$$

and extracting certain asymptotic and normalisation data, known as the 'scattering data', from the eigenfunction $\psi(x,k)$. The remarkable discovery made in [GGKM67] consists of the fact that the evolution of the scattering data under the action of an explicitly known 1-parameter group, is sufficient in the case of KdV to give the solution $u(x,t)$ at any later time t. Zakharov and Faddeev were able to construct symplectic coordinates for the form ω^2 defined above, which depended *only* upon the differentials of the scattering data. They then went on to show that these coordinates play the role of action-angle coordinates with respect to the KdV Hamiltonian $H(u)$.

There is a well-developed perturbation theory of integrable equations, generally studied in the following context: write the original system in terms of the action-angle variables

$$\frac{\mathrm{d}\mathbf{I}}{\mathrm{d}t} = \mathbf{0}\,, \qquad \frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega(\mathbf{I})\,, \qquad \omega(\mathbf{I}) = \frac{\partial H}{\partial \mathbf{I}}\,,$$

and consider

$$\frac{\mathrm{d}\mathbf{I}}{\mathrm{d}t} = \varepsilon\mathbf{f}(\mathbf{I},\theta)\,, \qquad \frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega(\mathbf{I}) + \varepsilon\mathbf{g}(\mathbf{I},\theta)\,,$$

for $\varepsilon \ll 1$. This theory is basically limited to finite dimensions or to "compact" perturbations in infinite dimensions (e.g. [Pos90]). Unfortunately, this sort of perturbation holds no hope of encompassing the lattice equations for the following two reasons: first, the above is a perturbation of the *Hamiltonian* of KdV, whereas the comparison between KdV and FPU is a comparison of two *kinematically* different systems (both of which are infinite dimensional) and second the "distance" between Hamiltonians is infinite in the sense that each interatomic interaction is changed by a fixed amount and there is an infinity of such interactions.

[7]Note that the description of an integrable system previously given is for *finite* dimensional systems. However, the concept may be generalised (along with the concept of action-angle variables) to infinite dimensions [KP02]. Similarly, there also exists an infinite dimensional KAM Theorem, as long as attention is restricted to *finite* dimensional (i.e. 'quasi'-periodic as opposed to 'almost'-periodic) solutions.

1.4 Relation of the potentials to quantum mechanical theory

The choice of the spring potential in our lattice equations can have a large impact upon their physical validity. In this Section we explore some of the motivating factors in the choice of a potential where the chain is intended to model a long chain of nearest-neighbour coupled atoms.[8] To investigate the potential between two such atoms we shall require the following quantum mechanical Hamiltonian operators (displayed here in electrostatic units):

$$\widehat{H}_{\mathrm{PAIR}} = -\sum_{i=1}^{N_1+N_2} \frac{\hbar^2}{2m_e}\triangle_{r_i} - \sum_{i=1}^{N_1+N_2}\Big(\frac{Z_1e^2}{|r_i|} + \frac{Z_2e^2}{|r_i-R|}\Big) + \sum_{1\le i<j\le N_1+N_2} \frac{e^2}{|r_i-r_j|}\,,$$

$$\widehat{H}_1 = -\sum_{i=1}^{N_1} \frac{\hbar^2}{2m_e}\triangle_{r_i} - \sum_{i=1}^{N_1}\frac{Z_1e^2}{|r_i|} + \sum_{1\le i<j\le N_1} \frac{e^2}{|r_i-r_j|}\,,$$

$$\widehat{H}_2 = -\sum_{i=N_1+1}^{N_1+N_2} \frac{\hbar^2}{2m_e}\triangle_{r_i} - \sum_{i=N_1+1}^{N_1+N_2}\frac{Z_2e^2}{|r_i-R|} + \sum_{N_1+1\le i<j\le N_1+N_2} \frac{e^2}{|r_i-r_j|}\,.$$

These operators are associated with the energy of electrons orbiting fixed nuclei. The first operator represents the electronic energy in a diatomic molecule with nuclei clamped at positions 0 and R, whereas the second and third represent the electronic energies of the two dissociated atoms at these positions. The first atom (with dissociated Hamiltonian operator $\widehat{H}_1$) has N_1 electrons, while the second has N_2 electrons. The charge on the first nucleus is Z_1e and the charge on the second is Z_2e. $\triangle_{r_i}$ denotes the Laplacian with respect to the i^{th} position coordinate. The meaning of 'position coordinate' is described more fully below. In each of the operators, the first terms represent kinetic energy, the second terms represent the attraction of the electrons to the nuclei and the third terms represent the repulsion between electrons. The universal constants used are $\hbar$ (Planck's constant divided by 2π), m_e (the rest mass of an electron) and e (the charge on an electron).

[8]The physical importance of FPU chains stems, among other things, from the fact that they are expected to display some of the major properties of (complicated) biological molecules. Such molecules will in general differ in two ways from the FPU model investigated here: there may be 'side branches' off the main chain and the masses and potentials will not be homogeneous across the length of the chain (e.g. [Sal91]). However, it is likely that, even without such physical motivations, the complexity which is known to emerge from their apparent simplicity would be sufficient to make FPU chains an attractive field of study in its own right.

Let $\psi_{\text{PAIR}} = \psi_{\text{PAIR}}(r_1, s_1, \ldots, r_{N_1+N_2}, s_{N_1+N_2})$, $\psi_1 = \psi_1(r_1, s_1, \ldots, r_{N_1}, s_{N_1})$ and $\psi_2 = \psi_2(r_1, s_1, \ldots, r_{N_2}, s_{N_2})$ denote the wavefunctions of the electrons in the diatomic system, the first atomic system and the second atomic system, respectively. $r_i \in \mathbb{R}^3$ is the position of the i^{th} electron and $s_i \in \{-1/2, 1/2\} = \mathbb{Z}_2$ is its spin. We thus have $\psi_{\text{PAIR}} : (\mathbb{R}^3 \times \mathbb{Z}_2)^{N_1+N_2} \to \mathbb{C}$, $\psi_1 : (\mathbb{R}^3 \times \mathbb{Z}_2)^{N_1} \to \mathbb{C}$ and $\psi_2 : (\mathbb{R}^3 \times \mathbb{Z}_2)^{N_2} \to \mathbb{C}$. The Pauli Exclusion Principle for electrons stipulates that the wavefunctions must be anti-symmetric. They are also required to be normalised (in L^2) and to have a certain degree of smoothness (H^1 into $\mathbb{C}$).

To each such wavefunction there corresponds an energy. A quantum mechanical system with Hamiltonian operator $\widehat{H}$ will generally prefer to adopt the wavefunction giving the lowest, or 'ground state', energy. To find this energy we can minimize the L^2 inner product $\langle \psi \big| \widehat{H} \psi \rangle$ over all admissible functions

$$\mathcal{A} := \left\{ \psi \in H^1\big((\mathbb{R}^3 \times \mathbb{Z}_2)^K; \mathbb{C}\big) \;\middle|\; \|\psi\|_{L^2} = 1 \text{ and } \psi \text{ antisymmetric} \right\},$$

where K is chosen to allow compatibility with the operator $\widehat{H}$.

This procedure can now be used with the first and second dissociated atomic Hamiltonian operators to find the ground state energies of those atoms:

$$E^{(1)} = \min_{\psi \in \mathcal{A}} \langle \psi \big| \widehat{H}_1 \psi \rangle \,, \quad E^{(2)} = \min_{\psi \in \mathcal{A}} \langle \psi \big| \widehat{H}_2 \psi \rangle \,.$$

Before the same can be done with the diatomic system we must replace $\widehat{H}_{\text{PAIR}}$ by $\widehat{H}_{\text{PAIR}} + \widehat{V}_{nn}$, where $\widehat{V}_{nn} := e^2 Z_1 Z_2 / |R|$ represents the nucleus-nucleus repulsion. Having done this, we may now write

$$E^{(\text{PAIR})} = \min_{\psi \in \mathcal{A}} \langle \psi \big| (\widehat{H}_{\text{PAIR}} + \widehat{V}_{nn}) \psi \rangle \,.$$

The potential energy stored in the "spring" connecting the two atoms is now given by the energy of the diatomic system, $E^{(\text{PAIR})}$ minus the total energy $E^{(1)} + E^{(2)}$ of the two dissociated atoms. This quantity will depend only upon the parameter R.

Formal calculations suggest that there exists $R_0 > 0$ such that, if the ground state electron densities (i.e. wavefunctions) of the two dissociated atoms are radially symmetric, then $R > R_0$ implies that the spring potential is proportional to $1/|R|^6$ (see, for example, [Lav99]). This rate of decay in the binding of atoms is commonly known as Van der Waals law. On the other hand, it is known that the internuclear repulsion will send the potential to $+\infty$ rapidly in the limit $R \to 0$. Finally, experimentation and calculation confirm that we should expect a 'preferred separation' (referred to as 'equilibrium spacing') at which the potential energy takes a global minimum. For any

potential to be considered physically accurate we expect, at least, that these three aspects be obeyed.

It is clear that the FPU potential does *not* display either of the first two aspects. So, despite the fact that its simplicity makes it an attractive candidate in the study of nonlinear springs, it cannot be thought of as a good potential with which to model molecules. The Lennard-Jones potential is given (in terms of the displacement r from equilibrium spacing) by

$$V(r) = \mu \left[\left(1 + \frac{r}{\nu}\right)^{-12} - 2\left(1 + \frac{r}{\nu}\right)^{-6} + 1 \right] .$$

If R_e denotes equilibrium spacing, then to put the formula in terms of R we need only replace r by $|R| - R_e$. As $R \to \infty$ the leading order term will indeed be $|R|^{-6}$. By correctly choosing the parameter ν we can ensure a rapid blow-up at 0. Finally, the graph of the potential also displays a unique global minimum to the right of zero. Hence, we have good reason to believe that lattice equations based upon the Lennard-Jones potential will reflect some of the behaviour expected in long-chain molecules. The final potential which we shall mention is the Toda potential:

$$V(r) = \frac{\kappa}{\lambda} e^{-\lambda r} + \kappa r \, .$$

Although this does not display Van der Waals decay or rapid growth at zero, the Toda potential's most remarkable property is that, as discussed below, it gives rise to an integrable set of lattice equations.

1.5 Two non-generic cases

1.5.1 The linear lattice

We refer to the linear case as "non-generic" rather than "special", because it is in fact of a *different* type to that discussed in the remainder of this work. Indeed, the potential used in the linear case has, in the notation of (2.1) in the following Chapter, $\beta = 0$, a situation specifically precluded elsewhere. The fact that the linear case does not fall within the scope of the majority of this work emphasises the fundamental difference between the linear and non-linear models.

Returning to (1.1) and putting $\beta = 0$ gives the linear form of the equation:

$$\ddot{q}_i = \alpha(q_{i+1} - 2q_i + q_{i-1}) \, . \tag{1.6}$$

We hold the first and last lattice sites fixed by setting $q_0 = q_{N+1} = 0$. We shall specify initial conditions towards the end of the solution process. As a 'first attempt' at solving (1.6), we can put $q_i(t) = \Phi(i)\Theta(t)$. This leads to

$$\frac{1}{\alpha}\frac{\ddot{\Theta}(t)}{\Theta(t)} = \frac{\Phi(i+1) - 2\Phi(i) + \Phi(i-1)}{\Phi(i)} = \lambda\,,$$

where λ is a constant, necessarily independent from both t and i. We begin by attempting to solve

$$\Phi(i+1) - 2\Phi(i) + \Phi(i-1) = \lambda\Phi(i)\,. \tag{1.7}$$

Since the left-hand-side is strongly reminiscent of a second order derivative operator, we suggest the solution

$$\Phi(i) = C_1\sin(\lambda i) + C_2\cos(\lambda i)\,.$$

This will satisfy the boundary conditions if $C_2 = 0$ and $\lambda = \frac{k\pi}{N+1}$ for $k = 1, \ldots, N$. Hence,

$$\Phi(i) = C_1\sin\Big(\frac{k\pi}{N+1}i\Big)\,. \tag{1.8}$$

Clearly, (1.8) does not solve (1.7). This will not be a significant problem if we are able, nevertheless, to solve the central problem

$$\frac{1}{\alpha}\frac{\ddot{\Theta}(t)}{\Theta(t)} = \frac{\Phi(i+1) - 2\Phi(i) + \Phi(i-1)}{\Phi(i)}\,.$$

For this to be possible it is sufficient that the right-hand-side be independent of i. By use of some standard trigonometric identities we find that the right-hand-side may be written

$$-4\sin^2\Big(\frac{k\pi}{2(N+1)}\Big)\,.$$

Thus, the time equation to be solved is

$$\ddot{\Theta}(t) = -\omega_k^2\Theta(t)\,, \tag{1.9}$$

where

$$\omega_k = 2\sqrt{\alpha}\sin\Big(\frac{k\pi}{2(N+1)}\Big)\,. \tag{1.10}$$

Hence, $\Theta(t) = A_k\sin\omega_k t + B_k\cos\omega_k t$. We now impose the initial conditions

$$q_i^{(k)}(0) = C_k\sin\Big(\frac{k\pi}{N+1}i\Big)\,, \quad \dot{q}_i^{(k)}(0) = 0\,, \tag{1.11}$$

so that $A_k = 0$ and $B_k = (C_k/C_1)q_i^{(k)}(0)$. The solutions of (1.6) subject to (1.11) and zero boundary conditions are thus of the form

$$q_i^{(k)}(t) = C_k \sin\Big(\frac{k\pi}{N+1} i\Big) \cos \omega_k t \,. \tag{1.12}$$

These solutions are commonly called the 'normal modes' of the lattice. The natural motion of the lattice can be expressed as a superposition of these normal modes: $Q_i(t) := \sum_k q_i^{(k)}$. Note that the amplitude C_k of the k^{th} mode is fixed by the initial condition and that no energy transfer takes place between the modes.

To make explicit the lack of energy transfer in this linear case we may define the energy of the l^{th} mode to be

$$E_l = \frac{1}{2}(\dot{\eta_l}^2 + \omega_l^2 \eta_l^2) \,,$$

where η_l is the l^{th} normal coordinate, defined by

$$\eta_l = \frac{2}{N+1} \sum_{i=1}^{N} Q_i \sin\Big(\frac{l\pi}{N+1} i\Big) \,.$$

The total energy of the whole system is simply $E = \sum_l E_l$. One then finds by direct calculation that, if the initial data are given by (1.11), then $Q_i(t) = q_i^{(k)}(t)$ and the total energy in the lattice is given by $(1/2)C_k^2\omega_k^2$. This is true for all time (including $t = 0$) and we thus conclude that there is no energy sharing between modes.

Finally, we point out an interesting relationship between the dispersive nature of harmonic lattice waves and the group velocity. We use (1.10) in this modified form:

$$\omega_k = 2\sqrt{\alpha} \, \Big| \sin\Big(\frac{k\pi}{2(N+1)}\Big) \Big| \,,$$

which has physical meaning as a relation between wave number and frequency. Close to $k = 0$, the frequency is low and the wavelength is long. One would expect in this limit that there is little if any difference between the speed of transmission of energy as measured by $\mathrm{d}\omega_k/\mathrm{d}k$ as compared to the sonic speed of transmission in a continuum (given as $\sqrt{Y/\rho}$ for the wave equation $u_{xx} - (\rho/Y)u_{tt} = 0$ in a continuous bar with Young's modulus Y and mass density ρ). We suspect this on the basis of the fact that a long wavelength would tend to imply that the atoms are moving in phase with one another, as a rigid body movement. However, as k increases towards $N+1$ one finds that the value of $\mathrm{d}\omega_k/\mathrm{d}k$ drops off. This can be interpreted [Oma75] as a discreteness effect, because as the wavelength shortens neighbouring atoms will tend to move out of phase with one another. It is argued that this scatters the group transmission thus

slowing it down. The idea that the wavespeed tends to slow down as the discrete nature of the lattice becomes more important shall prove valuable when attempting to give physical meaning to discreteness effects in the nonlinear case.

1.5.2 The Toda lattice

We now deal with the remarkable case of the Toda lattice which is completely integrable in the sense that the equations of motion possess the same number of conserved quantities as there are lattice sites ([Fla74], [Man74], [Tod81]). The Toda lattice is a mass-spring chain with equation of motion of type (1.2), where we take

$$V(r) = \frac{\kappa}{\lambda} e^{-\lambda r} + \kappa r \, .$$

This potential has the following limiting behaviour:

- for $|r| \ll 1$, $V(r) \approx \kappa/\lambda + (\kappa\lambda/2)r^2$, which is the potential for a linear lattice;
- for $\lambda \gg 1$, we obtain the "hard sphere" limit of near-infinite repulsion, when r is small.

As usual, the equations of motion (1.2) may be written as

$$\ddot{r_i} = V'(r_{i+1}) - 2V'(r_i) + V'(r_{i-1}) \, . \tag{1.13}$$

However, it is commonplace when investigating properties of the Toda lattice to make the force $f_i := -V'(r_i)$ the subject of (1.13) and then to solve for f_i. We note that $f_i = \kappa(e^{-\lambda r_i} - 1)$ and that (1.13) may then be written

$$\partial_{tt}\big[\chi(f_i)\big] = -f_{i+1} + 2f_i - f_{i-1} \, , \tag{1.14}$$

where $\chi(f_i) := -(1/\lambda)\ln(f_i/\kappa + 1)$. One finds that the following expression for f_i solves (1.14):

$$f(i,t) := f_i = \frac{1}{\lambda} B^2 \mathrm{sech}^2(bi \pm Bt) \, , \tag{1.15}$$

where $B = B(b) = \sqrt{\kappa\lambda}\sinh b$ and where our definition of the function $f : \mathbb{Z} \times \mathbb{R} \to \mathbb{R}$ is intended to emphasise the analogy between the discrete variable i and the position variable of a continuum theory. (1.15) represents a solitary wave travelling along the lattice with speed

$$c = \sqrt{\kappa\lambda}\,\frac{\sinh b}{b} \, .$$

The long wavelength regime corresponds to the limit $b \to 0$. This gives a 'sonic speed' for the lattice of $\sqrt{\kappa\lambda}$. The solitary wave always travels faster than this critical speed

for $b \neq 0$. Such super-sonic travel is a feature common to all nonlinear lattice solitary wave solutions.

It was shown by Hirota [Hir73] that the Toda lattice actually supports *multi*-soliton solutions. The method used was, in essence, direct verification of the fact that a generalised form of the single soliton solution happens to solve (1.14). Hirota's solution may be written as

$$q_i(t) = \frac{\partial^2}{\partial t^2} \ln g(\theta)\,,$$

where g is a known function and $\theta = \Omega t - \Lambda i - \delta$. This form of solution is identical to that found by Hirota for the KdV equation [Hir71].

A more systematic way of obtaining multi-solitons (and indeed other solutions) is to use the Inverse Scattering Transform (IST), some details of which have already been touched upon (see Section 1.3). The success of the IST in relation to the Toda problem [Tes99] (and indeed in relation to the KdV equation as well) stems from the fact that the eigenvalues of an associated eigenvalue problem are independent of time as long as the 'potential' of the eigenvalue problem evolves according to (1.14).

As with all completely integrable systems, the Toda lattice possesses a large number of conserved quantities relative to its number of degrees of freedom. In the finite dimensional case, with $2N$ degrees of freedom[9], there are N conserved quantities. These have a fairly simple formulation in terms of the dependent variables of a recast version of the equations of motion. Write the equations of motion as

$$\begin{aligned} \dot{q_i} &= p_i \\ \dot{p_i} &= \kappa\big(e^{-(q_i - q_{i-1})} - e^{-(q_{i+1} - q_i)}\big)\,, \end{aligned} \tag{1.16}$$

where λ has been removed by a rescaling of q_i. These may then be recast as

$$\begin{aligned} \dot{X}_i &= (p_i - p_{i+1})X_i \\ \dot{p_i} &= X_{i-1} - X_i\,, \end{aligned}$$

where $X_i := \kappa e^{-(q_{i+1} - q_i)}$. It was demonstrated by Hénon [Hen74] that one way of writing the N conserved quantities of this system (and hence of the original Toda system) is

$$I_m = \sum p_{i_1} p_{i_2} \cdots p_{i_k} (-X_{j_1})(-X_{j_2}) \cdots (-X_{j_l})\,, \quad m = 1, 2, \ldots, N\,. \tag{1.17}$$

The summation is composed in the following way:

[9]Recall that a lattice with N lattice sites defines a $2N$-dimensional phase space.

1. the equality $m = k + 2l$ should hold;

2. the indices $i_1, \ldots, i_k, j_1, \ldots, j_l$ involved in a given product $p_{i_1} \cdots p_{i_k}(-X_{j_1}) \cdots (-X_{j_l})$ within the summation should all be different from one another and from any member of the set $\{j_1 + 1, \ldots, j_l + 1\}$;

3. a product within the summation is excluded if it is a simple re-ordering of another product within the same summation - i.e. only distinct products are included.

Despite the fact that (1.17) was derived for the periodic lattice, integrals very closely related to these turn out to be valid for the lattice with zero boundary conditions as well. Hénon goes on to demonstrate how, with only minor alterations, (1.17) is useful for predicting the integrals of the infinite lattice.

In their paper Sawada and Kotera [SK76] not only confirmed (in the finite dimensional case), using a more standard Hamiltonian approach, that (1.17) does define a full set of Toda lattice integrals, but also that *if* expressions of the form (1.17) were to be regarded as integrals of a lattice system, then that system *must* be the Toda system. In particular, they showed that a Toda lattice potential is a necessary condition in order to guarantee that $(A, \bar{H}) = 0$, where the left-hand-side denotes the Poisson bracket of a quantity A of form (1.17) with the Hamiltonian

$$\bar{H} := \frac{1}{2} \sum_i p_i^2 + \left(\bar{V}(q_{i+1} - q_i) + \bar{V}(q_i - q_{i-1}) \right).$$

Note that this is an alternative formulation of a 'Toda-type' Hamiltonian. For example, taking $\bar{V}(r) := -\kappa e^{-r}$ gives (1.16) as Hamilton's equations of motion. The Poisson bracket discussed here is the standard finite dimensional Poisson bracket, defined by

$$(F, G) = \sum_i \frac{\partial G}{\partial p_i} \frac{\partial F}{\partial q_i} - \frac{\partial G}{\partial q_i} \frac{\partial F}{\partial p_i},$$

for any two functions F, G in the canonical coordinate space $\mathbb{R}^{2n} = \{(\mathbf{p}, \mathbf{q})\}$. See below for an explanation of why this is a genuine Poisson bracket in the sense of the definition of page 6.

Returning to the Toda integrals and noting that $\bar{V}'(q_{i+1} - q_i) = -\bar{V}'(q_i - q_{i+1})$, the Poisson bracket $(A, \bar{H})$ may be expressed in terms of the operator

$$\mathcal{H} := \sum_i p_i \frac{\partial}{\partial q_i} - \left(\bar{V}'(q_i - q_{i+1}) + \bar{V}'(q_i - q_{i-1}) \right) \frac{\partial}{\partial p_i}$$

on A:

$$\mathcal{H}A = (A, \bar{H}),$$

so that the general equation of motion may be written $\dot{A} = \mathcal{H}A$. A necessary condition on $\bar{V}$ is then sought in order to ensure $\dot{A} \equiv 0$. The Toda potential emerges after some calculation as the only possibility (see [SK76] for details).

The 'Poisson bracket' discussed above is now reconciled with the earlier definition. The finite dimensional expression for (F, G) given above is produced from the more general definition $(F, G) = \omega^2(I\mathrm{d}F, I\mathrm{d}G)$, when the symplectic structure ω^2 is given by $\omega^2(\xi, \eta) := J\xi \cdot \eta$, for any ξ, $\eta \in \mathbb{R}^{2n}$, where

$$J := \begin{pmatrix} 0 & -E^n \\ E^n & 0 \end{pmatrix}$$

(E^n the $n \times n$ identity matrix). I denotes the isomorphism between 1-forms and vector fields. By a standard result from Hamiltonian mechanics (for example [Arn89], p.215) we have $\omega^2(I\mathrm{d}F, I\mathrm{d}G)(x) = \mathrm{d}/\mathrm{d}t\big|_{t=0} F\big(g_G^t(x)\big)$, where g_G^t is the phase flow of G. Standard results ([Arn89], p.216) also establish that this more general bracket, and hence also its special case, do indeed satisfy the Leibniz rule and the Jacobi identity as set out on page 6. Hence, the 'Poisson bracket' used in this Subsection is a genuine Poisson bracket and we may properly call G a Hamiltonian function.

1.6 Recent developments and plan of the work

The fact that large dimensional lattice equations do not fall within the domain of applicability of standard perturbation theory (since the infinite dimensional perturbation would have to be kinematic in nature[10] and since the total difference between 'perturbed' and 'unperturbed' interactions is infinity across the whole lattice) has meant that a distinct body of literature for such equations has emerged. The dominant concern is the characterisation of the effect of discreteness on solutions obtained by the use of a continuum limit (such as KdV) of the lattice equations. Examples from the physics literature include [Col81], [Ros86] where the lattice's finite difference operator is approximately inverted. Of particular motivational interest is the work in [FPP89], [Lee] which reveals the existence of 'radiation' in the lattice solution, a phenomenon not encountered in the integrable continuum limit.

[10] In this context, a kinematic perturbation is one for which the phase spaces of the perturbed and unperturbed problems are *qualitatively* different - in this case an uncountable space versus a countable one.

Advances in the mathematics of lattice solutions in recent years have included a variationally based proof that coherent modes (solitary waves) do indeed exist on the lattice, for generic interatomic potentials (although the initial conditions used were non-generic) [FW94]. The result is achieved by minimizing kinetic energy subject to a prescribed average potential energy for the lattice. The wave speeds of the resulting waves are not known explicitly by this technique. A complementary paper by Smets and Willem [SW97] achieves a similar result, but using a different functional and a *prescribed* wavespeed for solutions, which emerge as the critical points of the functional.

A recent paper by Iooss [Ioo00] gave a constructive method for obtaining *all* 'small' bounded travelling waves on the FPU lattice with generic potentials. It used a process of centre manifold reduction set out first in the context of small bounded solutions on lattices in the previous paper [IK00].

Finally, Friesecke and Pego [FP99] have shown that, in the (sufficiently slow) supersonic long-wave regime, lattice solitary waves lie close to KdV solitons. Moreover, [FP02] reduces the question of long-time stability for lattice solitary waves to long-time stability of an appropriately linearized equation. Proving stability for this linearized equation is the objective of future work in this area.

In this work we shall follow the approach taken in [FP99] which, generally speaking, allows the most 'direct' way of analysing and visualising lattice profiles, in terms of known evolution equations. The motivation for this work, as mentioned above, is based heavily upon the phenomenon of lattice radiation. This phenomenon, which has been observed in the wake of the interaction of two lattice solitary waves, is believed to be a genuine effect of discreteness. To understand it mathematically we must:

- quantify the effect of discreteness rigorously, and
- find an evolution law for lattice solitary waves.

These two concerns form the straight-forward structure of this work: Chapter 2 addresses the first concern, while the Chapter 3 addresses the second.

In Chapter 2 we will formally derive an equation whose solution captures, to first order, the discreteness effects of the lattice. We shall prove that it possesses a unique even solution, making it a good candidate for the correction to the KdV soliton approximation discussed in [FP99]. In Theorem 2.2 we shall prove that the solution obtained from our candidate equation is indeed the next order correction to the KdV soliton by showing that the error is $o(\varepsilon^4)$. The proof shall rely upon three technical

results (to be found in the Appendix), one of which is essentially a new 'quantitative' version of the Implicit Function Theorem. A numerical solution of our correction equation will be given. The contents of Chapter 2, together with the technical results of the Appendix have been published in *Nonlinearity* (see [McM02]).

Chapter 3 will use a formal argument to derive an evolution equation for soliton corrections. The equation will be, in effect, a time-dependent generalisation of the correcting equation found in Chapter 2. We shall go on to show that our evolution equation possesses a unique solution, at least for finite time, giving meaning to its numerical simulation. The proof will be effected through a semi-group theory approach. The numerical scheme used for the numerical simulation will be discussed and the results presented. Finally, we shall review some numerical methods which could offer viable alternatives to the one chosen. It is the author's intention to publish the majority of the contents of Chapter 3 as a 10 to 15 page article.

The importance of this work lies in the fact that it sheds light upon how discreteness effects are experienced by lattice solitons. It quantifies the extent of these effects upon interacting solitons and draws close parallels with other fields of work. Finally, it places the problem in a Hamiltonian context - something that has been an underlying theme of this introduction. The Hamiltonian context helps to connect this work to a larger body of literature and a wider field of study. Given the 'direct' approach which is taken in the derivation of the many of the equations in the forthcoming Chapters, this is something that may otherwise have been lacking. It is also hoped that a Hamiltonian perspective on FPU lattice equations helps to convey another aspect of their mathematical richness.

Chapter 2

Quantifying Discreteness on the Solitary Wave

2.1 Introducing the nonlinear problem

As indicated in the last Section, this Chapter is concerned with quantifying the "difference" between KdV solitons and the true lattice solitary waves. The approach taken is very much in the spirit of [FP99]. By a rigorous expansion, we are able to find the determining equation for the correction to the KdV soliton in the long-wave regime and ascertain the order of the remaining error. The equation (an ODE) is then solved numerically to give a profile which one should imagine as being added (with an appropriate reduction in its amplitude) to the KdV soliton profile. The result is a coherent mode with a slightly wider and (in one case) lower amplitude profile than that resulting from KdV alone.

We study the behaviour of solitary waves in one-dimensional lattices with the Hamiltonian

$$H = \sum_{j=-\infty}^{\infty} \left(\frac{1}{2} p(j)^2 + V\big(q(j+1) - q(j)\big) \right) ,$$

where $q(j)$ and $p(j)$ denote the displacement and momentum of the j^{th} lattice site. Note also that all particles in the lattice (or 'mass-spring chain') are considered to have equal mass and this mass is taken to be 1 and that we are concerned with the case where relative displacements from equilibrium decay at $\pm\infty$. The potential V is of a general type, satisfying the following hypotheses:

$$V \in C^6(\mathbb{R};\mathbb{R}) , \quad V(0) = V'(0) = 0 ,$$

$$V''(0) =: \alpha > 0 , \quad V'''(0) =: \beta \neq 0 , \quad V''''(0) =: \gamma . \tag{2.1}$$

Thus, we are in general dealing with a non-integrable infinite dimensional system. Hamilton's equations of motion yield $\partial_t q = p$ and

$$\partial_t p(t,j) = \big(\partial_t^2 q(t,j) =\big)\, V'\big(q(t,j+1) - q(t,j)\big) - V'\big(q(t,j) - q(t,j-1)\big)\,.$$

Letting $r(t,j) := q(t,j+1) - q(t,j)$ denote the distortion of the j^{th} bond length out of equilibrium (i.e. the relative displacement of adjacent lattice sites) the equation of motion becomes

$$\partial_t^2 r = (e^{\partial} - 2 + e^{-\partial})V'(r)\,, \tag{2.2}$$

where e^{∂} and $e^{-\partial}$ denote the shift operators along the lattice, defined by $e^{\partial} r(t,j) := r(t,j+1)$ and $e^{-\partial} r(t,j) := r(t,j-1)$. The potentials V to be considered in the following Sections as 'prototypes' were all introduced in Chapter 1:

1. the cubic FPU potential

$$V(r) = \frac{1}{2}\alpha r^2 + \frac{1}{6}\beta r^3\,;$$

2. the Lennard-Jones potential

$$V(r) = \mu\left[\left(1+\frac{r}{\nu}\right)^{-12} - 2\left(1+\frac{r}{\nu}\right)^{-6} + 1\right]\,;$$

3. the Toda potential

$$V(r) = \frac{\kappa}{\lambda}e^{-\lambda r} + \kappa r\,.$$

Considerably less attention will be paid to the last of these due to its 'non-generic' nature.

2.2 The fixed point formulation and formal results

In this Section we set out Friesecke and Pego's [FP99] new method for obtaining a continuum limit to the lattice equations. It involves the use of a fixed point representation of (2.2) in terms of a Fourier multiplier. We begin by looking for travelling waves moving with wave speed c:

$$r_c(j - ct) := r(t,j)$$

so that (2.2) becomes

$$c^2\, r_c{}''(x) = (e^{\partial} - 2 + e^{-\partial})V'\big(r_c(x)\big)\,, \tag{2.3}$$

where $x := j - ct$. We may also write the restoring force as

$$V'(r) = \alpha r + N_1(r)\,,$$

where $N_1(r)$ denotes the non-linear part of the restoring force:

$$N_1(r) = \frac{\beta}{2} r^2 + \frac{\gamma}{3!} r^3 \big(1 + \eta(r)\big)\,,$$

where $\eta \in C^2(\mathbb{R};\mathbb{R})$ and $\eta(0) = 0$. For example, in the FPU case, $\gamma = 0$.

Thus, (2.3) becomes

$$c^2\, r_c{}''(x) = (e^{\partial} - 2 + e^{-\partial}) \left(\alpha r_c + N_1(r_c)\right). \tag{2.4}$$

Fourier transforming both sides of (2.4) (with the Fourier transform[1] defined by $\widehat{f}(\xi) := \int_{\mathbb{R}} e^{-ix\xi} f(x)\mathrm{d}x$) leads to

$$\left(c^2\,\xi^2 - 4\alpha \sin^2(\xi/2)\right) \widehat{r_c}(\xi) = 4\alpha \sin^2(\xi/2)\, \widehat{N(r_c)}(\xi)\,, \tag{2.5}$$

where $N(r_c) := N_1(r_c)/\alpha = \frac{\beta}{2\alpha} r_c^2 + \frac{\gamma}{3!\alpha} r_c^3 (1 + \eta(r_c))$. If $c > \sqrt{\alpha}$, $c^2\,\xi^2 - 4\alpha \sin^2(\xi/2)$ is one signed and non-zero. So, in that case, (2.5) can be written in the form of a fixed point equation:

$$r_c = P_c N(r_c) \tag{2.6}$$

where $P_c(\cdot) := \mathcal{F}^{-1}\left[\, p_c(\xi)\, \mathcal{F}(\cdot)\right]$ is the Fourier multiplier with symbol

$$p_c(\xi) = \frac{\alpha\, \mathrm{sinc}^2(\xi/2)}{c^2 - \alpha\, \mathrm{sinc}^2(\xi/2)}\,,$$

$\mathcal{F}$ (and $\mathcal{F}^{-1}$) denote the Fourier transform (and inverse Fourier transform) operators and $\mathrm{sinc}(z) = \sin(z)/z$.

We set

$$c = \sqrt{\alpha} \left(1 + \frac{\varepsilon^2}{24}\right)\,, \tag{2.7}$$

noting that $c = \sqrt{\alpha} = \sqrt{V''(0)}$ happens to be the maximum group velocity of the harmonic wave packets $\{e^{i(kx - \omega t)}\}_{\omega = \omega(k)}$.

Define ϕ by

$$\phi(\cdot) := (1/\varepsilon^2)\, r_c\,(\cdot/\varepsilon)\,.$$

[1]Here and in the rest of this work, significant use is made of the Fourier transform. Details concerning the range of applicability and derivative and difference formulae connected with this transform may be found in [LL01]. Where not explicitly stated/proved, such as in the formal arguments of Section 3.2, it is assumed that all functions belong to spaces on which the transform is well-defined and on which the relevant formulae may be used.

Changing variables from r_c to ϕ in (2.6) then leads to

$$\phi = P_c^{(\varepsilon)} N^{(\varepsilon)}(\phi) \tag{2.8}$$

where

$$P_c^{(\varepsilon)}(\cdot) := \mathcal{F}^{-1}\left[\frac{\varepsilon^2 \alpha \operatorname{sinc}^2(\varepsilon\xi/2)}{c^2 - \alpha \operatorname{sinc}^2(\varepsilon\xi/2)} \mathcal{F}(\cdot)\right],$$

and

$$N^{(\varepsilon)}(\phi) := \frac{\beta}{2\alpha}\phi^2 + \varepsilon^2 \frac{\gamma}{3!\alpha}\phi^3\left(1 + \eta(\varepsilon^2\phi)\right).$$

We shall also use the expression

$$N^{(\varepsilon)}(\phi) = \frac{\beta}{2\alpha}\phi^2\left(1 + \overline{\eta}(\varepsilon^2\phi)\right)$$

where $\overline{\eta} \in C^3$ and $\overline{\eta}(0) = 0$. Again, the existence of such a function $\overline{\eta}$ follows from the smoothness assumptions on V.

Next denote by $\phi_0 := (\alpha/4\beta)\operatorname{sech}^2(x/2)$ the nontrivial, up-to-translation-unique solution of the KdV equation

$$-\frac{\mathrm{d}}{\mathrm{d}x}u + 12(\beta/\alpha)\, u\left(\frac{\mathrm{d}}{\mathrm{d}x}u\right) + \frac{\mathrm{d}^3}{\mathrm{d}x^3}u = 0, \tag{2.9}$$

subject to $u \to 0$ as $|x| \to \infty$. As suggested above, the solution ϕ_0 is the lowest order non-vanishing approximation to the true solution of the lattice problem (2.6). This is proven in [FP99]. The proof relies, in particular, on the surprising fact that the first term in the formal Taylor series expansion of the symbol $p_c^{(\varepsilon)}(\xi) := \varepsilon^2 p_c(\varepsilon\xi)$ for small ε is a valid approximation for $p_c^{(\varepsilon)}$ *over all* $\xi \in \mathbb{R}$, and not just in the region of a priori validity - namely $\xi < \mathcal{O}(1/\varepsilon)$. The relevant result is [FP99] Corollary 3.4:

$$\sup_{\xi\in\mathbb{R}} |p_c^{(\varepsilon)}(\xi) - p^{(0)}(\xi)| \leq C\varepsilon^2,$$

where $p^{(0)}(\xi) := 12/(1+\xi^2)$. $p^{(0)}$ also defines the obvious Fourier multiplier $P^{(0)}(\cdot) := \mathcal{F}^{-1}p^{(0)}(\xi)\mathcal{F}(\cdot)$. Similarly, we shall also use the notation $N^{(0)}(\phi) = \beta/(2\alpha)\phi^2$. It is straight-forward to demonstrate the equivalence of $P^{(0)}N^{(0)}(\phi) = \phi$ and equation (2.9). In particular, we therefore have

$$\frac{12}{1+\xi^2}\left(\frac{\beta}{2\alpha}\widehat{\phi_0^2}\right) = \widehat{\phi_0}. \tag{2.10}$$

We now require a candidate for the correction and so we look for a candidate determining equation. This may be obtained formally by returning to (2.6) and making the appropriate multiscale substitution, which in this case is

$$r_c(\cdot) = \varepsilon^2\phi_0(\varepsilon\cdot) + \varepsilon^4\phi_1(\varepsilon\cdot).$$

The equation picked up at order ε^2 is (after some algebra) the following:

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}u + \big(3\,\mathrm{sech}^2(x/2) - 1\big)u = -\frac{\alpha}{320\beta}\mathrm{sech}^2(x/2) - \frac{\alpha}{16\beta}\mathrm{sech}^4(x/2) + \frac{\alpha}{32\beta}\big(3 - (\alpha\gamma/\beta^2)\big)\mathrm{sech}^6(x/2)\,, \qquad (2.11)$$

subject to $u \to 0$ as $|x| \to \infty$.

2.2.1 Existence and uniqueness of the steady state correction

In order for (2.11) to be a plausible/useful correcting equation, it must at least be shown to have a unique solution on the function space in which the lowest order approximation to (2.8) resides.[2] This function space is the even subspace of $H^1(\mathbb{R})$.[3]

Lemma 2.1. *Equation* (2.11) *has a unique even solution in* $H^1(\mathbb{R})$.

Proof. Write (2.11) in the equivalent form

$$\left(1 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)^{-1}\big(3\,\mathrm{sech}^2(x/2)u\big) - u = \left(1 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)^{-1} f\,, \qquad (2.12)$$

where f is defined to be the right-hand-side of (2.11). We begin by looking for *any* $H^1(\mathbb{R})$ solution to (2.12). It is manifest from (2.11) that any such solution will be smooth and will satisfy the stated boundary conditions. Under these conditions, the eigenfunction problem $(L - \lambda)u = 0$ where $Lu := \big(1 - \mathrm{d}^2/\mathrm{d}x^2\big)^{-1}\big(3\,\mathrm{sech}^2(x/2)u\big)$, is known in the literature (see [MF53], p.768 and Lemma 4.2 of [FP99]) and $\lambda = 1$ is known to be an eigenvalue. Moreover, the corresponding, unique, eigenfunction is

$$\psi(x) := \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{4}\,\mathrm{sech}^2(x/2)\right)$$

[2]Since publication of this material, it has been pointed out that (2.11) has, in fact, an explicit analytic solution. This can be seen to be the case by virtue of the fact that the following three relations hold for the operator $\bar{L} := \mathrm{d}^2/\mathrm{d}x^2 + 3\mathrm{sech}^2(x/2) - 1$:

- $\bar{L}\Big(\mathrm{sech}^2(x/2)\big(1 - (x/2)\tanh(x/2)\big)\Big) = \mathrm{sech}^2(x/2)$;
- $\bar{L}\big((2/3)\mathrm{sech}^2(x/2)\big) = \mathrm{sech}^4(x/2)$;
- $\bar{L}\Big(\mathrm{sech}^2(x/2)\big(1 - (1/2)\mathrm{sech}^2(x/2)\big)\Big) = \mathrm{sech}^6(x/2)$.

Each of the functions on the left-hand-side is even and tends to 0 as $x \to \pm\infty$.

[3]As in [FP99], we restrict to the even subspace in order to remove translational degeneracy.

- see [FP99] and [MF53]. This is an odd function. Now,

$$\langle \psi \, , \left(1 - \mathrm{d}^2/\mathrm{d}x^2\right)^{-1} f \rangle_{H^1} = \frac{1}{2\pi} \int_{-\infty}^{\infty} (1+|\xi|^2) \widehat{\psi} (1+|\xi|^2)^{-1} \overline{\widehat{f}} = \int_{-\infty}^{\infty} \psi f = 0$$

since f is an even function. Since L is a compact self-adjoint linear operator on $H^1(\mathbb{R})$ (see Lemma 4.2 of [FP99]), the Fredholm Alternative (see, for example, [Ped99]) is applicable and we find that (2.12) - and therefore (2.11) - is soluble. Moreover, the Fredholm Alternative also tells us that any solution takes the form

$$s = u_0 + a\psi$$

where u_0 is any solution to (2.11) and a is an arbitrary real number. Finally, by restricting attention to *even* functions only, we obtain a unique solution: we require $s(-x) = s(x)$ so that the only possibility for ψ is (using the fact that ψ is odd) $\psi(x) = (1/2a)\left(u_0(-x) - u_0(x)\right)$ and hence the non-uniqueness of s through adding multiples of ψ is lost. □

2.3 The rigorous expansion

We now show that the even $H^1(\mathbb{R})$ solution to (2.11) is indeed the discreteness-induced correction to the KdV soliton.

Let ϕ_1 denote the unique even solution to (2.11). It will prove useful to note that the decay in $\phi_1(x)$ as $|x| \to \infty$ must be exponential: since ϕ_1 decays, $3\mathrm{sech}^2(x/2)\,\phi_1$ must decay exponentially. Similarly, the right-hand-side of (2.11) decays exponentially. These facts force $\phi_1'' - \phi_1$ to decay exponentially also and this is only possible if ϕ_1 itself decays exponentially.

It was shown in [FP99] that for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, with ε_0 sufficiently small, there exists a unique even $H^1(\mathbb{R})$ solution $\phi^{(\varepsilon)}$ to (2.8). The following Theorem holds for the map $\varepsilon \mapsto \phi^{(\varepsilon)}$:

Theorem 2.2. *The map $\varepsilon^2 \mapsto \phi^{(\varepsilon)}$ is differentiable into $H^1(\mathbb{R})$ so that*

$$\frac{\|\phi^{(\varepsilon)} - \phi_0 - \varepsilon^2 (\mathrm{d}/\mathrm{d}\varepsilon^2)|_{\varepsilon^2=0} \phi^{(\varepsilon)}\|_{H^1(\mathbb{R})}}{\varepsilon^2} \to 0 \, , \tag{2.13}$$

as $\varepsilon^2 \to 0$. Moreover, $\mathrm{d}/\mathrm{d}\varepsilon^2 \big|_{\varepsilon^2=0} \phi^{(\varepsilon)} \equiv \phi_1$ and so we may write

$$\frac{\|\phi^{(\varepsilon)} - \phi_0 - \varepsilon^2 \phi_1\|_{H^1(\mathbb{R})}}{\varepsilon^2} \to 0 \, , \tag{2.14}$$

as $\varepsilon^2 \to 0$*, or, in terms of* r_c*,*

$$\frac{\|r_c(\cdot) - \varepsilon^2\phi_0(\varepsilon\cdot) - \varepsilon^4\phi_1(\varepsilon\cdot)\|_{L^\infty(\mathbb{R})}}{\varepsilon^4} \to 0\,, \tag{2.15}$$

as $\varepsilon^2 \to 0$*, where* $c = \sqrt{\alpha}(1 + \varepsilon^2/24)$*.*

The proof of the Theorem relies heavily upon Lemma A.1 which is to be found in the Appendix. This result may be viewed as the estimate which underlies any potential smoothness of an implicitly defined function, and is in this sense a quantitative version of the Implicit Function Theorem (for example, [Jos97]).

Other results which are used are Lemmas A.2 and A.3, also in the Appendix. From these we obtain the following: the map

$$(\varepsilon^2, \phi) \mapsto N^{(\varepsilon)}(\phi) = \frac{\beta}{2\alpha}\,\phi^2\left(1 + \overline{\eta}(\varepsilon^2\phi)\right)$$

is Fréchet differentiable in both arguments. To prove this, note that Lemma A.2 gives that $\varepsilon^2\phi \mapsto \overline{\eta}(\varepsilon^2\phi)$ is Fréchet differentiable from $H^1(\mathbb{R})$ into $H^1(\mathbb{R})$. Furthermore, Lemma A.3 implies that the map $(\phi, \varepsilon^2\phi) \mapsto N^{(\varepsilon)}(\phi)$ is also Fréchet differentiable from $H^1(\mathbb{R}) \times H^1(\mathbb{R})$ into $H^1(\mathbb{R})$. The result now follows since $(\varepsilon^2, \phi) \mapsto \varepsilon^2\phi$ is $C^\infty(\mathbb{R} \times H^1(\mathbb{R}); H^1(\mathbb{R}))$.

Proof. We define $F(\phi) := P^{(0)}N^{(0)}(\phi)$ and $\tilde{F}^{(\varepsilon)}(\phi) := P^{(\varepsilon)}N^{(\varepsilon)}(\phi) - P^{(0)}N^{(0)}(\phi)$. It is not difficult to see that both F and $\tilde{F}^{(\varepsilon)}$ are Gâteaux differentiable on all of $H^1(\mathbb{R})$ with bounded derivatives. Clearly, $\tilde{F}^{(0)}(\phi) = 0$ and by (2.10) we have $F(\phi_0) = \phi_0$. By the result in [FP99] already mentioned, we also have for ε sufficiently small $\tilde{F}^{(\varepsilon)}(\phi^{(\varepsilon)}) + F(\phi^{(\varepsilon)}) = \phi^{(\varepsilon)}$.

Define $S := \{\psi \in H^1(\mathbb{R}) : \psi(x)$ decays exponentially as $|x| \to 0\}$. Then, $\phi_0 \in S$ and also $\phi_{\mathrm{cor}} \in S$, if ϕ_{cor} is defined as prescribed in Lemma A.1. The first of these claims is clear, whereas the second arises from the fact that $\phi_{\mathrm{cor}} \equiv \phi_1$, where ϕ_1 is the unique even solution to (2.11), which decays exponentially. To see that $\phi_{\mathrm{cor}} \equiv \phi_1$ it is first necessary to verify that the map $\varepsilon^2 \mapsto \tilde{F}^{(\varepsilon)}(\phi_0)$ is differentiable at $\varepsilon^2 = 0$ and establish what the derivative is.

Define

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0}\tilde{F}^{(\varepsilon)}(\phi_0) := \mathcal{F}^{-1}\,p_1(\xi)\,\widehat{N^{(0)}(\phi_0)} + \mathcal{F}^{-1}\,p^{(0)}(\xi)\,\mathcal{F}\Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0}N^{(\varepsilon)}(\phi_0)\Big)\,,$$

where

$$p_1(\xi) := -\frac{3/5\,\xi^4 + \xi^2 + 1/2}{(1+\xi^2)^2}$$

is the second term in the formal Taylor series expansion of $p_c^{(\varepsilon)}$ and therefore offers a valid approximation to $p_c^{(\varepsilon)} - p^{(0)}$ whenever $\xi \in (-k/\varepsilon, k/\varepsilon)$ for all $k > 0$. So,

$$\begin{aligned}
&\Big\| \tilde{F}^{(\varepsilon)}(\phi_0) - \tilde{F}^{(0)}(\phi_0) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0) \Big\|^2_{H^1(\mathbb{R})} \\
&= \int_{\mathbb{R}} (1+\xi^2) \Big| p_c^{(\varepsilon)} \widehat{N^{(\varepsilon)}(\phi_0)} - p^{(0)} \widehat{N^{(0)}(\phi_0)} \\
&\quad - \varepsilon^2 p_1(\xi)\, \widehat{N^{(0)}(\phi_0)} - \varepsilon^2 p^{(0)}(\xi)\, \mathcal{F}\Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} N^{(\varepsilon)}(\phi_0) \Big) \Big|^2 d\xi
\end{aligned}$$

$$\begin{aligned}
&\leq 2 \int_{\mathbb{R}} (1+\xi^2) \Big| p^{(0)} \widehat{N^{(\varepsilon)}(\phi_0)} - p^{(0)} \widehat{N^{(0)}(\phi_0)} - \varepsilon^2 p^{(0)}(\xi)\, \mathcal{F}\Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} N^{(\varepsilon)}(\phi_0) \Big) \Big|^2 d\xi \\
&+ 2 \int_{\mathbb{R}} (1+\xi^2) \Big| p_c^{(\varepsilon)} \widehat{N^{(\varepsilon)}(\phi_0)} - p^{(0)} \widehat{N^{(\varepsilon)}(\phi_0)} - \varepsilon^2 p_1(\xi)\, \widehat{N^{(\varepsilon)}(\phi_0)} \Big|^2 d\xi \\
&+ 2 \int_{\mathbb{R}} (1+\xi^2) \Big| \varepsilon^2 p_1(\xi)\, \widehat{N^{(\varepsilon)}(\phi_0)} - \varepsilon^2 p_1(\xi)\, \widehat{N^{(0)}(\phi_0)} \Big|^2 d\xi
\end{aligned}$$

(The presence of the factors 2 is due to the fact that $|a+b|^2 \leq 2(|a|^2 + |b|^2)$, for all a, $b > 0$.) The first and last of these three integrals is indeed $o(\varepsilon^4)$, due to the continuity and differentiability of the map $\varepsilon^2 \mapsto N^{(\varepsilon)}(\phi_0)$. To see that the second integral is also $o(\varepsilon^4)$ we split it up as follows:

$$\begin{aligned}
&\int_{\mathbb{R}} (1+\xi^2) \Big| \big(p_c^{(\varepsilon)} - p^{(0)} - \varepsilon^2 p_1 \big) \widehat{N^{(\varepsilon)}(\phi_0)} \Big|^2 d\xi \\
&\quad = \int_{\mathrm{IN}(\varepsilon)} (1+\xi^2) \Big| \big(p_c^{(\varepsilon)} - p^{(0)} - \varepsilon^2 p_1 \big) \widehat{N^{(\varepsilon)}(\phi_0)} \Big|^2 d\xi \\
&\quad + \int_{\mathrm{OUT}(\varepsilon)} (1+\xi^2) \Big| \big(p_c^{(\varepsilon)} - p^{(0)} - \varepsilon^2 p_1 \big) \widehat{N^{(\varepsilon)}(\phi_0)} \Big|^2 d\xi
\end{aligned}$$

where $\mathrm{IN}(\varepsilon)$ denotes the inner region $(-k/\varepsilon, k/\varepsilon)$ and $\mathrm{OUT}(\varepsilon)$ denotes the outer region $(-\infty, -k/\varepsilon] \cup [k/\varepsilon, \infty)$. Since $\sup_{\xi \in \mathrm{IN}(\varepsilon)} |p_c^{(\varepsilon)} - p^{(0)} - \varepsilon^2 p_1|$ is $o(\varepsilon^2)$, the first of these integrals poses no problem. For the second we have

$$\begin{aligned}
&\int_{\mathrm{OUT}(\varepsilon)} (1+\xi^2) \Big| \big(p_c^{(\varepsilon)} - p^{(0)} - \varepsilon^2 p_1 \big) \widehat{N^{(\varepsilon)}(\phi_0)} \Big|^2 d\xi \\
&\quad \leq 16 \sup_{\xi \in \mathbb{R}} \big(|p_c^{(\varepsilon)}(\xi) - p^{(0)}(\xi)|^2 + \varepsilon^4 |p_1(\xi)|^2 \big) \int_{\mathbb{R}} (1+\xi^2) \Big| \widehat{N^{(\varepsilon)}(\phi_0)} - \widehat{N^{(0)}(\phi_0)} \Big|^2 d\xi \\
&\quad + 16 \sup_{\xi \in \mathbb{R}} \big(|p_c^{(\varepsilon)}(\xi) - p^{(0)}(\xi)|^2 + \varepsilon^4 |p_1(\xi)|^2 \big) \int_{\mathrm{OUT}(\varepsilon)} (1+\xi^2) \Big| \widehat{N^{(0)}(\phi_0)} \Big|^2 d\xi
\end{aligned}$$

Therefore, given that

$$\sup_{\xi \in \mathbb{R}} |p_c^{(\varepsilon)}(\xi) - p^{(0)}(\xi)| \leq C\varepsilon^2 \,,$$

and $\varepsilon^2 \mapsto N^{(\varepsilon)}(\phi_0)$ is a continuous map there remains only to show that

$$\int_{\mathrm{OUT}(\varepsilon)} (1+\xi^2) \Big| \widehat{N^{(0)}(\phi_0)} \Big|^2 \, d\xi \to 0$$

as $\varepsilon^2 \to 0$. This is true by virtue of the fact that ϕ_0 and therefore $N^{(0)}(\phi_0)$ is an exponentially decaying function (which is enough to ensure a sufficiently fast decay in Fourier space).

The assertion that $\phi_{\mathrm{cor}} \equiv \phi_1$ now follows because the determining equation for ϕ_{cor} is

$$A\phi_{\mathrm{cor}} = \phi_{\mathrm{cor}} - DF(\phi_0)\phi_{\mathrm{cor}} = \mathcal{F}^{-1}\, p_1(\xi)\, \widehat{N^{(0)}(\phi_0)} + \mathcal{F}^{-1}\, p^{(0)}(\xi)\, \mathcal{F}\Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} N^{(\varepsilon)}(\phi_0) \Big) .$$

Alternatively, in Fourier space (for all $\xi \in \mathbb{R}$)

$$\widehat{\phi_{\mathrm{cor}}} - \frac{12}{1+\xi^2}\, \frac{\beta}{\alpha}\, \widehat{\phi_0 \phi_{\mathrm{cor}}} = -\frac{3/5\xi^4 + \xi^2 + 1/4}{(1+\xi^2)^2}\, \frac{\beta}{2\alpha}\, \widehat{\phi_0^2} + \frac{12}{1+\xi^2}\, \frac{\gamma}{3!\alpha}\, \widehat{\phi_0^3} ,$$

or, equivalently,

$$(1+\xi^2)\widehat{\phi_{\mathrm{cor}}} - \frac{12\beta}{\alpha}\widehat{\phi_0\phi_{\mathrm{cor}}} = -(3/5\xi^4 + \xi^2 + 1/4)\frac{\widehat{\phi_0}}{12} + 12\frac{\gamma}{3!\alpha}\widehat{\phi_0^3} , \tag{2.16}$$

using the fact that $P^{(0)}N^{(0)}(\phi_0) = \phi_0$. This is exactly the equation which ϕ_1 satisfies (this can be checked by carrying out the Fourier inversion of (2.16) and then performing the differentiations of the known function ϕ_0 on the right-hand-side). Hence, $\phi_{\mathrm{cor}} \equiv \phi_1 \in S$.

The condition of differentiability of $\varepsilon^2 \mapsto \tilde{F}^{(\varepsilon)}(\phi)$ at $\varepsilon^2 = 0$ for all $\phi \in S$ can now be fulfilled by repeating the above argument proving differentiability of $\varepsilon^2 \mapsto \tilde{F}^{(\varepsilon)}(\phi_0)$ at $\varepsilon^2 = 0$, but replacing ϕ_0 by any $\phi \in S$.

The remaining conditions (invertibility of A and the boundedness properties 1 and 2 on the derivatives $DF(\phi)$ and $D\tilde{F}^{(\varepsilon)}(\phi)$) were proven in [FP99]. In particular, 1 follows by the fact that F is smooth on $H^1(\mathbb{R})$ and 2 follows from the fact that $\|D\tilde{F}^{(\varepsilon)}(\phi)\|_{H^1(\mathbb{R})\to H^1(\mathbb{R})} \leq C\varepsilon^2$, for C independent of ε. The result now follows easily from estimate (A.2) of Lemma A.1. Note that the final term in (A.2) is indeed $o(\varepsilon^2)$ since $\mathrm{d}/\mathrm{d}\varepsilon^2\,\big|_{\varepsilon^2=0}\tilde{F}^{(\varepsilon)}(\cdot)$ is continuous on S. This follows from the fact that $\mathrm{d}/\mathrm{d}\varepsilon^2\,\big|_{\varepsilon^2=0}N^{(\varepsilon)}(\cdot)$ is continuous on S - a fact that is easy to verify since $\mathrm{d}/\mathrm{d}\varepsilon^2\,\big|_{\varepsilon^2=0}N^{(\varepsilon)}(\phi) = \gamma/(3!\alpha)\,\phi^3$. □

2.4 Numerical results and interpretation

Equation (2.11) may be discretised using the standard finite-difference method and solved numerically. By rescaling the independent (time) and dependent (amplitude) variables in (2.2) we may 'choose' the values of α and β (as long as $\alpha > 0$ and $\beta \neq 0$). Once this has been done, the value of γ is automatically determined by the underlying form of the potential. In fact, in the FPU case $\gamma = 0$ irrespective of the values of α and β. If we take $\alpha = \beta = 1$ in the Lennard-Jones case, however, we force $\gamma = 53/63$. A few numerical simulations are presented below. It should also be noted that since physical springs are typically hard against compression but soft against expansion, one should expect such a spring to possess a potential energy with $\beta < 0$. Thus, $\alpha = 1$, $\beta = -1$ should be regarded as the physical situation. In the Lennard-Jones case (as well as in the FPU case, of course) γ remains unaltered by the change in the sign of β. These physical plots are not shown as they are simply given by the reflection of the non-physical profiles in the x-axis.

Figure 2.3 shows that the profile of the corrected FPU soliton lies just above the KdV soliton and displays a distinct widening of its base compared to KdV. Nevertheless, the agreement between KdV and corrected soliton is very high. On the other hand, Figure 2.4 indicates that the Lennard-Jones profile (which involves a higher order nonlinearity) shows a slightly larger mismatch with KdV, particularly close to its maximum, where the profile dips below KdV. It also displays a widening of its base. The comparison between the uncorrected and the corrected soliton in the Lennard-Jones case, in particular, is reminiscent of the comparison between a fast KdV soliton and a slow KdV soliton (respectively). The parallel seems particularly appropriate in light of the considerations relating to dispersion of waves on the linear lattice put forward on page 15. It would appear that increasing the importance of the lattice in wave propagation tends, if not to slow the wave down, then at least to give it the *profile* of a slower wave.

It is also interesting to point out one major difference between Figures 2.1 and 2.2: the FPU profile is positive across all space, whereas the Lennard-Jones profile becomes negative close to zero. This is therefore a *qualitative* difference between when a higher order nonlinearity is included as opposed to when it is not ($\gamma \neq 0$ versus $\gamma = 0$). A qualitative difference (in fact between existence and non-existence of solitary waves) is also observed when the case $\beta \neq 0$ is compared with $\beta = 0$.

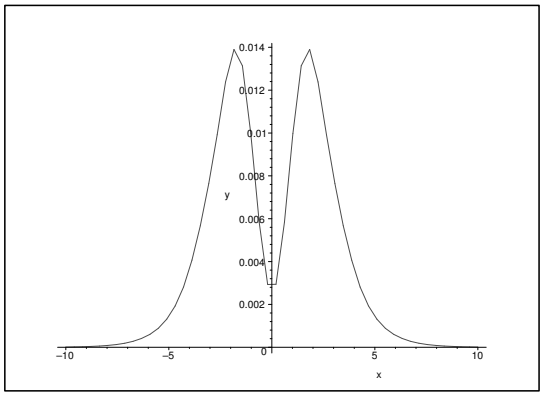


Figure 2.1: The FPU correction profile

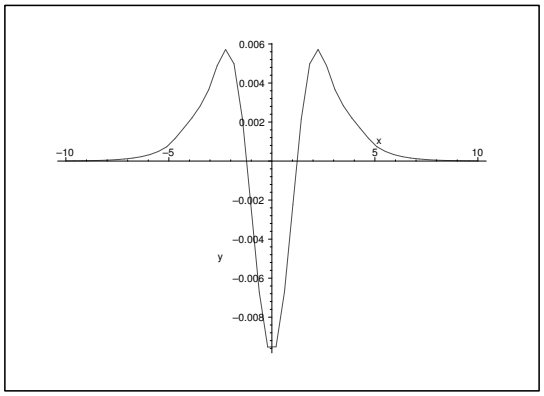


Figure 2.2: The Lennard-Jones correction profile

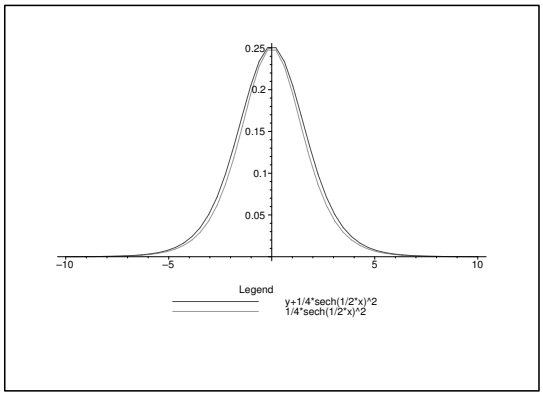


Figure 2.3: The KdV soliton and corrected FPU soliton with $\varepsilon = 1$

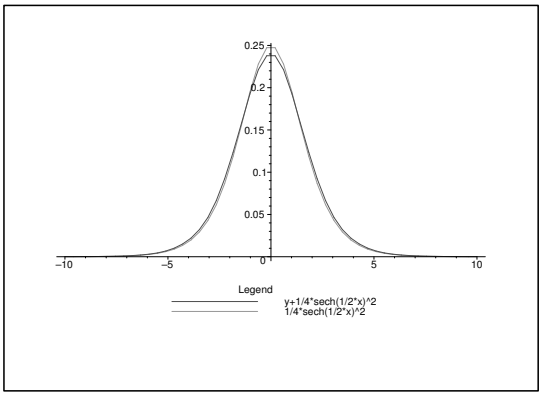


Figure 2.4: The KdV soliton and corrected Lennard-Jones soliton with $\varepsilon = 1$

Finally, we point out a particularly intriguing aspect of (2.11): its effective independence from γ for all prototype potentials. That is to say, although the final term on the right-hand-side of (2.11) contains γ, it turns out that 'fixing' the values of α and β in either the Lennard-Jones or the Toda potential automatically determines γ's dependence on α and β; the particular form of this dependence negates the right-hand-side's perceived dependence upon γ. Explicitly, we find

$$\gamma = C\beta^2/\alpha\,, \tag{2.17}$$

with $C = 53/63$ for Lennard-Jones and $C = 1$ for Toda. It is now clear that the product $\alpha\gamma/\beta^2$ which appears in the final term of (2.11) is simply a constant independent of the choice of α and β. The same is evidently also true in a trivial sense for the

FPU potential. We find that the solution to (2.11) depends in an effective way only upon the ratio α/β.

This aspect fits well with the fact that the solution to (2.11) is intended to correct the soliton solution to (2.9), whose amplitude also depends exclusively upon the ratio α/β, because it implies that the amplitude of the correction varies linearly with that of the soliton. Of course, the relation (2.17) is in some sense 'obvious' (or at least 'necessary') for *all* potentials because otherwise it would imply that the correction were dependent upon how the independent and dependent variables in (2.2) are rescaled, which is absurd.

Chapter 3

The Effects of Discreteness

3.1 Introduction

As mentioned in the introduction, there is now considerable evidence to suggest that one of the effects of discreteness upon lattice solutions is the development of 'radiation' as a result of the interaction of two lattice solitons. This phenomenon is indeed thought to be an effect of discreteness because it is not displayed by the integrable KdV equation which models the continuum limit. In this Chapter we hope to account for the radiation by observing how the correction to a *bi*soliton evolves. The intention is to demonstrate that the lattice radiation is indeed a 'higher-order' discreteness effect.

To achieve this goal, it is first necessary to propose the evolution equation for the bisoliton correction. The Section 3.2 deals with how we obtain such an equation. For this to be a *viable* candidate we also need to demonstrate the existence and uniqueness of solutions with appropriate properties. This is done in the Section 3.3. Finally, Sections 3.4, 3.5 and 3.6 are given over to the numerical simulation of the evolution equation and examination of the output.

3.2 Evolution of the bisoliton correction

To obtain a candidate for the bisoliton correction we take an approach reminiscent of the previous Chapter and we begin with the generic FPU lattice equation (1.2):

$$\partial_t^2 r(i,t) = (e^{\partial} - 2 + e^{-\partial})(\alpha\, r(i,t) + (\beta/2)\, r^2(i,t) + (\gamma/3!)\, r^3(i,t) + \cdots)\,.$$

As before, we are concerned with lattices of particles whose relative displacements from equilibrium vanish at $\pm\infty$. Note that here we have assumed that the potential

is sufficiently smooth to allow its expansion to the required number of terms. Since we are looking for a solution with two travelling waves we make the substitution

$$r(i,t) = \phi(\theta_1, \theta_2)\,, \tag{3.1}$$

where $\theta_1 := i - c_1 t$ and $\theta_2 := i - c_2 t$. Then,

$$\begin{aligned} c_1^2\,\phi_{11}(\theta_1,\theta_2) + 2\,c_1\,c_2\,\phi_{12}(\theta_1,\theta_2) + c_2^2\,\phi_{22}(\theta_1,\theta_2) \\ = (e^{\partial} - 2 + e^{-\partial})(\alpha\phi + (\beta/2)\phi^2 + (\gamma/3!)\phi^3 + \cdots)\,, \end{aligned}$$

where ϕ_{11} denotes the derivative of ϕ with respect to its first component twice, with the similar meanings for ϕ_{12} and ϕ_{22}, and where the symbolic notation e^{∂} and $e^{-\partial}$ is now given by

$$e^{\partial}\phi(\theta_1,\theta_2) = \phi(\theta_1+1,\theta_2+1), \qquad e^{-\partial}\phi(\theta_1,\theta_2) = \phi(\theta_1-1,\theta_2-1)\,.$$

Fourier transforming with respect to θ_1 and then θ_2 gives

$$\begin{aligned} -c_1^2\xi_1^2\widehat{\widehat{\phi}}(\xi_1,\xi_2) - 2c_1c_2\widehat{\widehat{\phi}}(\xi_1,\xi_2) - c_2^2\xi_2^2\widehat{\widehat{\phi}}(\xi_1,\xi_2) \\ = -4\sin^2\Big(\frac{\xi_1+\xi_2}{2}\Big)(\alpha\widehat{\widehat{\phi}}(\xi_1,\xi_2) + (\beta/2)\widehat{\widehat{\phi^2}}(\xi_1,\xi_2) + \cdots)\,. \end{aligned}$$

This leads to

$$\widehat{\widehat{\phi}}(\xi_1,\xi_2) = \frac{4\alpha\sin^2\big((\xi_1+\xi_2)/2\big)}{(c_1\xi_1+c_2\xi_2)^2 - 4\alpha\sin^2\big((\xi_1+\xi_2)/2\big)}\Big(\frac{\beta}{2\alpha}\widehat{\widehat{\phi^2}} + \cdots\Big)\,.$$

We now introduce the small parameter ε by making the following substitution:

$$\phi(\theta_1,\theta_2) =: \varepsilon^2\phi_0(\varepsilon\theta_1,\varepsilon\theta_2) + \varepsilon^4\phi_1(\varepsilon\theta_1,\varepsilon\theta_2)\,.$$

The Fourier space equation then becomes

$$\begin{aligned} &\widehat{\widehat{\phi}}_0(\xi_1,\xi_2) + \varepsilon^2\widehat{\widehat{\phi}}_1(\xi_1,\xi_2) \\ &= \frac{4\varepsilon^2\alpha\sin^2\big((\varepsilon\xi_1+\varepsilon\xi_2)/2\big)}{(c_1\varepsilon\xi_1+c_2\varepsilon\xi_2)^2 - 4\alpha\sin^2\big((\varepsilon\xi_1+\varepsilon\xi_2)/2\big)}\Big(\frac{\beta}{2\alpha}\widehat{\widehat{\phi}}_0^2 + \varepsilon^2\frac{\beta}{\alpha}\widehat{\widehat{\phi_0\phi_1}} + \varepsilon^2\frac{\gamma}{3!\alpha}\widehat{\widehat{\phi}}_0^3 + \mathcal{O}(\varepsilon^4)\Big)\,. \end{aligned} \tag{3.2}$$

We again make use of ε by specifying that the wavespeeds c_1 and c_2 be given by

$$c_1 = \sqrt{\alpha}\Big(1 + \frac{\varepsilon^2}{24}\mu_1\Big), \qquad c_2 = \sqrt{\alpha}\Big(1 + \frac{\varepsilon^2}{24}\mu_2\Big)\,,$$

for some fixed $\mu_1,\ \mu_2 > 0$. It is now possible to expand the prefactor on the right-hand-side of (3.2) in terms of ε and collect together terms with the same order in ε.

After some manipulation this gives the following order zero and order 2 equations, respectively:

$$\widehat{\widehat{\phi_0}} = \frac{12(\xi_1+\xi_2)}{\mu_1\xi_1+\mu_2\xi_2+(\xi_1+\xi_2)^3}\frac{\beta}{2\alpha}\widehat{\widehat{\phi_0^2}}\,, \tag{3.3}$$

$$\begin{aligned}\widehat{\widehat{\phi_1}} = {} & \frac{12(\xi_1+\xi_2)}{\mu_1\xi_1+\mu_2\xi_2+(\xi_1+\xi_2)^3}\Big(\frac{\beta}{\alpha}\widehat{\widehat{\phi_0\phi_1}}+\frac{\gamma}{3!\alpha}\widehat{\widehat{\phi_0^3}}\Big) \\ & - \frac{(1/4)(\mu_1\xi_1+\mu_2\xi_2)^2+(\mu_1\xi_1+\mu_2\xi_2)(\xi_1+\xi_2)^3+(3/5)(\xi_1+\xi_2)^6}{(\mu_1\xi_1+\mu_2\xi_2)^2+2(\mu_1\xi_1+\mu_2\xi_2)(\xi_1+\xi_2)^3+(\xi_1+\xi_2)^6}\Big(\frac{\beta}{2\alpha}\widehat{\widehat{\phi_0^2}}\Big)\,.\end{aligned} \tag{3.4}$$

The programme is now as follows: equations (3.3) and (3.4) are Fourier transformed back into real space to obtain equations in terms of θ_1 and θ_2, where θ_1 and θ_2 are the new "continuum versions" of the old (lattice based) θ_1, θ_2 coordinates. At this stage we shall effect a change of variables from θ_1, θ_2 to another pair of continuum variables x and t (yet to be defined). These will be chosen in such a way as to put the real-space version of (3.3) into the standard KdV form. Before carrying out the first stage of this programme (the Fourier transform), however, it is convenient (although not necessary) to effect part of the change of coordinates whilst still in Fourier space:

$$\xi_1 \mapsto \frac{\sqrt{\mu_1}}{2}\,\xi_1, \qquad \xi_2 \mapsto \frac{\sqrt{\mu_2}}{2}\,\xi_2\,.$$

The order zero equation then transforms back in to real coordinates to give the following:

$$\frac{1}{8}(\sqrt{\mu_1}\partial_{\theta_1}+\sqrt{\mu_2}\partial_{\theta_2})^3\phi_0+\frac{6\beta}{\alpha}\phi_0(\sqrt{\mu_1}\partial_{\theta_1}+\sqrt{\mu_2}\partial_{\theta_2})\phi_0-\frac{1}{2}(\mu_1^{3/2}\partial_{\theta_1}+\mu_2^{3/2}\partial_{\theta_2})\phi_0=0\,. \tag{3.5}$$

This is just the KdV equation

$$u_{xxx}+6uu_x+u_t=0 \tag{3.6}$$

with double travelling wave ansatz

$$u(x,t)=\phi_0(\theta_1,\theta_2)\,,$$

where

$$\theta_1=a_1x-4a_1^3t, \qquad \theta_2=a_2x-4a_2^3t\,, \tag{3.7}$$

with

$$a_1=\Big(\frac{\alpha\mu_1}{8\beta}\Big)^{1/2}, \qquad a_2=\Big(\frac{\alpha\mu_2}{8\beta}\Big)^{1/2}.$$

Note that (3.7) implicitly defines our new coordinates x and t. (3.6) is known to have the solution

$$u(\theta_1,\theta_2) = 2\frac{\partial^2}{\partial x^2}\ln f(x,t) \tag{3.8}$$

where $f(x,t) := 1+\exp(2\theta_1)+\exp(2\theta_2)+A\exp(2\theta_1+2\theta_2)$, θ_1 and θ_2 as above and $A := \big((a_1-a_2)/(a_1+a_2)\big)^2$. See [Hir71].

We now turn to the real space version of (3.4). Factorising the denominator of the second prefactor in (3.4) allows us to make use of (3.3) to obtain

$$\widehat{\widehat{\phi}}_1 = \frac{12\big((\mu_1^{1/2}/2)\,\xi_1+(\mu_2^{1/2}/2)\,\xi_2\big)}{(\mu_1^{3/2}/2)\,\xi_1+(\mu_2^{3/2}/2)\,\xi_2+\big((\mu_1^{1/2}/2)\,\xi_1+(\mu_2^{1/2}/2)\,\xi_2\big)^3}\Big(\frac{\beta}{\alpha}\widehat{\widehat{\phi_0\phi_1}}+\frac{\gamma}{3!\alpha}\widehat{\widehat{\phi_0^3}}\Big)-\frac{\varphi}{\varrho}\Big(\widehat{\widehat{\phi}}_0\Big)\,, \tag{3.9}$$

where

$$\begin{aligned}\varphi :=&(1/4)\big((\mu_1^{3/2}/2)\,\xi_1+(\mu_2^{3/2}/2)\,\xi_2\big)^2\\ &+\big((\mu_1^{3/2}/2)\,\xi_1+(\mu_2^{3/2}/2)\xi_2\big)\big((\mu_1^{1/2}/2)\,\xi_1+(\mu_2^{1/2}/2)\,\xi_2\big)^3\\ &+(3/5)\big((\mu_1^{1/2}/2)\,\xi_1+(\mu_2^{1/2}/2)\,\xi_2\big)^6\end{aligned}$$

and

$$\begin{aligned}\varrho :=&\Big((\mu_1^{3/2}/2)\,\xi_1+(\mu_2^{3/2}/2)\,\xi_2+\big((\mu_1^{1/2}/2)\,\xi_1+(\mu_2^{1/2}/2)\,\xi_2\big)^3\Big)\\ &\cdot\Big(12\big((\mu_1^{1/2}/2)\xi_1+(\mu_2^{1/2}/2)\xi_2\big)\Big)\,.\end{aligned}$$

We bring the right-hand-side of (3.9) together over a common denominator and transform back into real space. We then change the variables from θ_1, θ_2 to the x, t of the KdV equation (3.6) by defining derivatives as follows:

$$\partial_x^n\phi = \Big(\sqrt{\frac{\alpha}{2\beta}}\big((\sqrt{\mu_1}/2)\partial_{\theta_1}+(\sqrt{\mu_2}/2)\partial_{\theta_2}\big)\Big)^n\phi$$

and

$$\partial_t^m\phi = \Big(-\big(\frac{\alpha}{2\beta}\big)^{3/2}\big((\mu_1^{3/2}/2)\partial_{\theta_1}+(\mu_2^{3/2}/2)\partial_{\theta_2}\big)\Big)^m\phi\,,$$

as was done when transforming (3.5) into (3.6). The order two correcting equation can then be written

$$\partial_x^4\phi_1+6\partial_x^2(\phi_0\phi_1)+\partial_t\partial_x\phi_1 = \frac{\beta}{6\alpha}\big((1/4)\partial_t^2+\partial_t\partial_x^3+(3/5)\partial_x^6\big)\phi_0-\frac{\gamma}{\beta}\partial_x^2(\phi_0^3)\,.$$

Recalling that the KdV bisoliton ϕ_0 is itself an x derivative we may integrate this equation up once in x to get

$$\partial_x^3\phi_1+6\partial_x(\phi_0\phi_1)+\partial_t\phi_1 = \frac{\beta}{24\alpha}\partial_t^2\Phi_0+\frac{\beta}{6\alpha}\partial_t\partial_x^2\phi_0+\frac{\beta}{10\alpha}\partial_x^5\phi_0-\frac{\gamma}{\beta}\partial_x(\phi_0^3)+C(t)\,, \tag{3.10}$$

where $\Phi_0 := \int_{-\infty}^{x} \phi_0$ and $C(t)$ is an arbitrary function of t alone. By making use of the fact that ϕ_0 satisfies the KdV equation (3.6), it is possible to eliminate all t derivatives from the right-hand-side of (3.10) to get

$$\partial_x^3\phi_1+6\partial_x(\phi_0\phi_1)+\partial_t\phi_1 = \frac{1}{2\alpha\beta}(\beta^2-2\alpha\gamma)\partial_x(\phi_0^3)-\frac{\beta}{2\alpha}\phi_0\partial_x^3\phi_0-\frac{\beta}{40\alpha}\partial_x^5\phi_0-\frac{9\beta}{8\alpha}\partial_x\big((\partial_x\phi_0)^2\big)\,. \tag{3.11}$$

Here $C(t)$ was identically equated to zero by assuming suitable zero boundary conditions. It is reassuring to note that (3.11) reduces to the real space version of (2.16) (that is to say equation (2.11)), when the travelling wave substitution

$$\theta = 2(ax - 4a^3t - \delta)\,,$$

with $a := (\alpha/8\beta)^{1/2}$ and δ fixed, is used along with relationship (2.9) for ϕ_0. It is not difficult to see that this is exactly the substitution required to return from the x, t coordinates to the θ coordinate of the continuum limit, when $\mu = 1$.

Although (3.11) was obtained by use of a "double travelling wave" substitution (see (3.1)) it is clear that the same equation would be obtained if we had used instead a "multiple travelling wave" substitution. We may conclude that (3.11) is a candidate correction equation for the KdV multisoliton on the lattice. However, it is the usefulness of (3.11) for determining the evolution of the correction to the *bi*soliton that shall concern us in this work.

In general terms, (3.11) may be viewed as an evolution equation for discreteness effects on the lattice. It is interesting to note that it is itself a linearised KdV equation with a non-zero forcing term. An equation of this type is also thought to govern the evolution of the correction to the KdV soliton in shallow water wave theory - [Lai60], [AI77] and [Joh97] - and in the theory of ion-acoustic waves [IMK76]. It is remarkable that the same equation (albeit with a different forcing term) appears to play the same rôle in generic FPU theory - where the correction is due primarily to lattice discreteness rather than to nonlinear effects.

For comparison, we note the corresponding equations in shallow water wave theory and ion-acoustic theory, respectively:

- $\partial_x^3\phi_1 + 6\partial_x(\phi_0\phi_1) + \partial_t\phi_1 = 3/2\Big(12\partial_x(\phi_0^3) + 12\phi_0\partial_x^3\phi_0 + \partial_x^5\phi_0 + 9\partial_x\big((\partial_x\phi_0)^2\big)\Big)$;
- $\partial_x^3\phi_1 + 6\partial_x(\phi_0\phi_1) + \partial_t\phi_1 = 2^{1/3}\Big(18\phi_0\partial_x\phi_0 - (9/2)\partial_x^5\phi_0 - (45/2)\partial_x\big((\partial_x\phi_0)^2\big)\Big)$.

The similarity with the equation from shallow water wave theory is particularly striking. This equation differs from our own only by the numeric coefficients in the forcing term.

With regard to the domain of definition and initial conditions of our equation, we note that since (3.11) is intended to correct a KdV equation it should ideally be defined on the time interval $[-\infty, \infty]$, with initial data given at $t = -\infty$, as is the case with the standard KdV equation. Essentially the initial data should be of the form

$$\phi_0(x, -\kappa) = \phi_{\mathrm{CORR}}(x + 4a_1^2\kappa) + \phi_{\mathrm{CORR}}(x + 4a_2^2\kappa + (1/2)\ln A)\,, \quad \kappa \to \infty \qquad (3.12)$$

where ϕ_{CORR} denotes the correction to the single soliton, given by the solution to equation (2.11). The shift terms $4a_1^2\kappa$ and $4a_2^2\kappa + (1/2)\ln A$ ensure that at $\kappa = \infty$ the two corrections will lie exactly above the two single solitons making up the bisoliton solution at $t = -\infty$. See [MH86] for the asymptotic positions of the solitons in a bisoliton solution. The precise form of the initial data will be given in Section 3.4.

3.3 Existence and uniqueness of solutions

In this Section we prove, using a semigroup-theoretic approach, that our candidate equation (3.11), subject to the initial condition of type (3.12) and zero boundary conditions, has a unique classical solution, at least for *finite* time. Our problem may be given as follows:

$$\begin{array}{rcll} \mathrm{d}\bar{u}(\tau)/\mathrm{d}\tau & = & \bar{A}(\tau)\bar{u}(\tau) + \bar{f}(\tau)\,, & -\kappa \le \tau \le T \\ \bar{u}(-\kappa) & = & u_0\,, & \end{array} \qquad (3.13)$$

where we have adopted the new notation $\bar{u}$, τ in place of the old ϕ_1, t of (3.11) and where $T > -\kappa$ is any fixed, finite, real number. $\bar{A}(\tau)$ is defined to be the time-dependent differential operator $-\big(\partial_x^3 + 6\phi_0(\tau)\partial_x + 6(\partial_x\phi_0(\tau))\big)$ and f denotes the right-hand-side of (3.11). For each given τ, $u(\tau)$ and $f(\tau)$ (and also u_0) are viewed as elements of an appropriate function space, to be defined below.

To obtain a problem which fits better with standard theory, it is convenient to shift (3.13) in such a way as to have the initial condition placed at zero time. To do this we define

$$t := \tau + \kappa\,, \qquad \bar{u}(\tau) =: u(t)\,, \qquad \bar{A}(\tau) =: A(t)\,, \qquad \bar{f}(\tau) =: f(t)\,.$$

(3.13) then becomes

$$\begin{array}{rcll} \mathrm{d}u(t)/\mathrm{d}t & = & A(t)u(t) + f(t)\,, & 0 \le t \le T + \kappa \\ u(0) & = & u_0\,, & \end{array} \qquad (3.14)$$

where

$$A(t) = -\big(\partial_x^3 + 6\phi_0(t-\kappa)\partial_x + 6(\partial_x\phi_0(t-\kappa))\big) \tag{3.15}$$

and

$$f(t) = \bar{f}(t-\kappa)\,. \tag{3.16}$$

In order to prove the existence and uniqueness of a solution to (3.14) in the case where κ is fixed and finite, it is sufficient to prove existence and uniqueness for the slightly modified problem

$$\begin{array}{rcll} \mathrm{d}u(t)/\mathrm{d}t & = & A(t)u(t) + f(t)\,, & 0 \le t \le T \\ u(0) & = & u_0\,, & \end{array} \tag{3.17}$$

where

$$A(t) = -\big(\partial_x^3 + 6\phi_0(t)\partial_x + 6(\partial_x\phi_0(t))\big) \tag{3.18}$$

and

$$f(t) = \bar{f}(t)\,. \tag{3.19}$$

This is true because if the hypotheses of Theorem 3.7 below are satisfied for the operator (3.18) and forcing term (3.19), then they are manifestly also satisfied for the operator (3.15) and forcing term (3.16). In other words, a finite time shift makes no difference.

Before we come to the Theorem which asserts the existence and uniqueness of a classical solution to (3.17), and consequently also to (3.13), we give some preliminary semigroup theoretic definitions and results, which may be found in [Paz83].

Definition 3.1. A family $\{T(t)\}_{0\le t\le T}$ of bounded operators on some Banach space X is called a C_0 *semigroup* if it satisfies the usual definitions of a semigroup and if each of the operators is *strongly continuous* i.e. for every $x \in X$, $\lim_{t\to 0} T(t)x = x$.

Theorem 3.2 (Fundamental Theorem for C_0 Semigroups). *Let $T(t)$ be a C_0 semigroup. Then, there exist constants $\omega \ge 0$ and $M \ge 1$ such that*

$$\|T(t)\| \le Me^{\omega t}\,,$$

for $0 \le t \le T$.

Definition 3.3. Let X be a Banach space and let $\{T(t)\}_{0\le t\le T}$ be a semigroup of bounded linear operators on X. An operator $L : D(L) \to X$ with domain

$$D(L) := \left\{ x \in X : \lim_{t\to 0} \frac{T(t)x - x}{t} \text{ exists} \right\}$$

which satisfies

$$Lx = \lim_{t \to 0} \frac{T(t)x - x}{t},$$

for $x \in D(L)$ is called the *infinitesimal generator* of the semigroup $T(t)$.

Hereafter, we shall use the notation $L \in \mathcal{G}(X, M, \omega)$ if L is the infinitesimal generator of a semigroup $T(t)$ which is C_0 and which satisfies $\|T(t)\| \leq Me^{\omega t}$.

Definition 3.4. Let X be a Banach space. A family of infinitesimal generators $A(t) : D\big(A(t)\big) \to X$ of C_0 semigroups on X is called *stable* if there are constants $M \geq 1$ and ω (called the *stability constants*) such that

$$\rho\big(A(t)\big) \supset]\omega, \infty[$$

for $t \in [0, T]$, and

$$\Big\| \prod_{j=1}^{k} R\big(\lambda : A(t_j)\big) \Big\| \leq M(\lambda - \omega)^{-k} \tag{3.20}$$

for $\lambda > \omega$ and every finite sequence $0 \leq t_1 \leq t_2 \leq \cdots \leq t_k \leq T$, $k = 1, 2, \ldots$. Here $\rho\big(A(t)\big)$ denotes the resolvent set for $A(t)$ and $R\big(\lambda : A(t)\big) := (\lambda I - A(t))^{-1}$. Note also that the product which appears on the left-hand-side of (3.20) consists of operators which do not in general commute. Hence the following convention is adopted: the operator $R(\lambda : A(t_i))$ shall stand to the left of the operator $R(\lambda : A(t_j))$ whenever $i \geq j$.

Remark 3.5. A sufficient condition for a family $\{A(t)\}_{0 \leq t \leq T}$ of operators to be stable is that for all $t \in [0, T]$, $A(t) \in \mathcal{G}(X, 1, \omega)$, i.e. $A(t)$ is the infinitesimal generator of a C_0 semigroup $S_t(s)$, $s \geq 0$ satisfying $\|S_t(s)\| \leq e^{\omega s}$. The stability constants in this case will be $M = 1$ and ω. This result originates from a simple Corollary to the Hille-Yosida Theorem (e.g. [Paz83] p.12). The Corollary states that the semigroup $S_t(s)$ satisfies the condition $\|S_t(s)\| \leq e^{\omega s}$ precisely if the generator $A(t)$ of the semigroup satisfies the following conditions:

- $A(t)$ is closed and $\overline{D\big(A(t)\big)} = X$;
- The resolvent set $\rho(A(t))$ of $A(t)$ contains the ray $\{\lambda : \mathrm{Im}\lambda = 0,\ \lambda > \omega\}$ and for such λ, $\|R\big(\lambda : A(t)\big)\| \leq (\lambda - \omega)^{-1}$.

Definition 3.6. Let X be a Banach space. A two parameter family of bounded linear operators $U(t, s)$, $0 \leq s \leq t \leq T$ on X is called an *evolution system* if the following three conditions hold:

- $U(s,s) = I$;
- $U(t,r)U(r,s) = U(t,s)$ for $0 \leq s \leq r \leq t \leq T$;
- $(t,s) \mapsto U(t,s)$ is strongly continuous for $0 \leq s \leq t \leq T$.

We now come to the central Theorem of this Section, which we shall make use of in solving our particular problem.

Theorem 3.7. *Let X be a Banach space. Suppose each member of the family $\{A(t)\}_{0\leq t\leq T}$ of time-dependent operators has domain $D(A(t)) =: D$, independent of t, and is a stable infinitesimal generator of a C_0 semigroup on X. Moreover, for all $v \in D$ let $t \mapsto A(t)v$ be continuously differentiable into X. Finally, let $f \in C^1\big([0,T];X\big)$. Then, the Banach space problem*

$$\begin{aligned} \mathrm{d}u(t)/\mathrm{d}t &= A(t)u(t) + f(t)\,, \qquad 0 \leq t \leq T \\ u(0) &= u_0 \in D\,, \end{aligned}$$

possesses a unique classical solution given by

$$u(t) = U(t,0)u_0 + \int_0^t U(t,r)f(r)\,\mathrm{d}r\,,$$

where $U : \mathbb{R}\times\mathbb{R} \to BL(X)$ is a uniquely determined evolution system. Here, $BL(X)$ denotes the set of bounded linear operators on X.

The proof of this Theorem can be found on p.147 of [Paz83].

In our case, we take $D(A(t)) := H^3(\mathbb{R})$, for all t, and $X := L^2(\mathbb{R})$. We are therefore required to check the following hypotheses:

1. $A(t)$ is stable;
2. $A(t)$ is an infinitesimal generator on $L^2(\mathbb{R})$;
3. for all $v \in H^3(\mathbb{R})$, the mapping $t \mapsto A(t)v$ is continuously differentiable into $L^2(\mathbb{R})$;
4. $f \in C^1\big([0,T];L^2(\mathbb{R})\big)$.

In checking these hypotheses, we shall make use of the following classical result from semigroup theory (e.g. [Paz83]):

Theorem 3.8 (Stone's Theorem). *L is the infinitesimal generator of a C_0 group of unitary operators on a Hilbert space H if and only if iL is self-adjoint.*

The two following perturbation results will also prove useful (e.g. [Paz83]):

Theorem 3.9. *Let $\{A(t)\}_{0\leq t\leq T}$ be a stable family of infinitesimal generators with stability constants M and ω. For $0 \leq t \leq T$, let $B(t)$ be bounded linear operators on X. If $\|B(t)\| \leq K$ for all $0 \leq t \leq T$, then $\{A(t) + B(t)\}_{t\in[0,T]}$ is a stable family of infinitesimal generators with stability constants M and $\omega + KM$.*

Theorem 3.10. *Let A be the infinitesimal generator of a C_0 semigroup of contractions. Let B be dissipative and satisfy $D(B) \supset D(A)$ and*

$$\|Bx\| \leq \alpha\|Ax\| + \beta\|x\|\,,$$

for $x \in D(A)$ where $0 \leq \alpha < 1$ and $\beta \geq 0$. Then, $A+B$ is the infinitesimal generator of a C_0 semigroup of contractions.

To prove hypothesis 1 write $A(t)$ as follows: $A(t) = A_0(t) + A_1(t)$ where $A_0(t) := -(\partial_x^3 + 6\phi_0(t)\partial_x)$ and $A_1(t) := -6\partial_x\phi_0(t)$. Suppose $A_0(t)$ were stable with stability constants 1 and ω and suppose $A_1(t)$ were a *bounded* linear operator on $L^2(\mathbb{R})$ with $\|A_1(t)\|_{L^2(\mathbb{R})\to L^2(\mathbb{R})} \leq K$, for all $0 \leq t \leq T$. Then it would follow, by Theorem 3.9 that $A_0(t) + A_1(t)$ is itself stable with stability constants 1 and $\omega + K$. Now, $A_1(t)$ is indeed bounded since if $\|\partial_x\phi_0(t)\|_{L^\infty(\mathbb{R})} \leq K/6$, say, then

$$\sup_{u\in L^2(\mathbb{R}),\, \|u\|\neq 0} \frac{\|A_1(t)u\|_{L^2(\mathbb{R})}}{\|u\|_{L^2(\mathbb{R})}} \leq \frac{6\|\partial_x\phi_0(t)\|_{L^\infty(\mathbb{R})}\|u\|_{L^2(\mathbb{R})}}{\|u\|_{L^2(\mathbb{R})}} \leq K\,.$$

So, it remains only to show that $A_0(t)$ is indeed stable with stability constants 1 and ω. By Remark 3.5 it suffices to show that $A_0(t) \in \mathcal{G}(X, 1, \omega)$.

Write $A_0(t) = B_0 + B_1(t)$ where $B_0 := -\partial_x^3$, $D(B_0) := H^3(\mathbb{R}) \subset L^2(\mathbb{R})$ and $B_1(t) := -6\phi_0(t)\partial_x$, $D(B_1(t)) := H^1(\mathbb{R}) \subset L^2(\mathbb{R})$. Now, if $u, v \in H^3(\mathbb{R})$, $\langle -\partial_x^3 u, v\rangle_{L^2(\mathbb{R})} = \langle u, \partial_x^3 v\rangle_{L^2(\mathbb{R})}$ so that $B_0^* = -B_0$ and hence iB_0 is self-adjoint on the Hilbert space $L^2(\mathbb{R})$. It now follows from Theorem 3.8 that B_0 is the infinitesimal generator of a C_0 group of unitary operators - i.e. the infinitesimal generator of a C_0 group of isometries. Hence, in particular, B_0 generates a C_0 semigroup of contractions on $L^2(\mathbb{R})$.

On the other hand, for $u \in H^1(\mathbb{R})$,

$$\langle -6\phi_0(t)\partial_x u, u\rangle_{L^2(\mathbb{R})} = -6\int_{\mathbb{R}} \phi_0(t)\partial_x u \cdot u = 6\int_{\mathbb{R}} \partial_x(\phi_0(t))|u|^2 + 6\int_{\mathbb{R}} \phi_0(t)u\partial_x u\,.$$

So, rearranging the second equality, we have

$$-12\int_{\mathbb{R}} \phi_0(t)\partial_x u \cdot u = 6\int_{\mathbb{R}} \partial_x(\phi_0(t))|u|^2\,.$$

Hence,

$$\langle -6\phi_0(t)\partial_x u, u\rangle_{L^2(\mathbb{R})} \leq 3\|\partial_x(\phi_0(t))\|^2_{L^\infty(\mathbb{R})} \int_{\mathbb{R}} |u|^2 \leq \frac{K^2}{12}\int_{\mathbb{R}} |u|^2 \,.$$

Denote $k := K^2/12$ so that we obtain

$$\langle B_1(t)u, u\rangle_{L^2(\mathbb{R})} - \langle ku, u\rangle_{L^2(\mathbb{R})} \leq 0\,,$$

i.e. $\big\langle (B_1(t)-k)u, u\big\rangle_{L^2(\mathbb{R})} \leq 0$. So, the operator $B_1(t)-k$ is dissipative over $L^2(\mathbb{R})$. Since $D(B_1(t)-k) \supset D(B_0)$, Theorem 3.10 will be applicable as long as there exist α and β such that $0 \leq \alpha < 1$, $\beta \geq 0$ with

$$\|(B_1(t)-k)u\|_{L^2(\mathbb{R})} \leq \alpha\|B_0 u\|_{L^2(\mathbb{R})} + \beta\|u\|_{L^2(\mathbb{R})}\,. \tag{3.21}$$

If the relative boundedness condition (3.21) holds, then Theorem 3.10 together with the above result about B_0, will imply that $B_0+B_1(t)-k$ is the infinitesimal generator of a C_0 semigroup of contractions. It will then follow that $B_0+B_1(t)$ is the infinitesimal generator of a C_0 semigroup $S_t(s)$, $s \geq 0$, with $\|S_t(s)\| \leq e^{kt}$, so that $A_0(t) \in \mathcal{G}(X, 1, k)$, as required.

To prove (3.21), note that for $u \in H^3(\mathbb{R})$,

$$\|(B_1(t)-k)u\|_{L^2(\mathbb{R})} \leq 6\|\phi_0(t)\|_{L^\infty(\mathbb{R})}\|\partial_x u\|_{L^2(\mathbb{R})} + k\|u\|_{L^2(\mathbb{R})}\,.$$

Now, for any $u \in H^3(\mathbb{R})$,

$$\|\partial_x u\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} |\partial_x u|^2 = -\int_{\mathbb{R}} \partial_x^2 u \cdot u \leq \|\partial_x^2 u\|_{L^2(\mathbb{R})}\|u\|_{L^2(\mathbb{R})}$$

and, moreover,

$$\|\partial_x^2 u\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} |\partial_x^2 u|^2 = -\int_{\mathbb{R}} \partial_x^3 u \cdot \partial_x u \leq \|\partial_x^3 u\|_{L^2(\mathbb{R})}\|\partial_x u\|_{L^2(\mathbb{R})}\,.$$

So,

$$\|\partial_x u\|^2_{L^2(\mathbb{R})} \leq \|\partial_x^3 u\|^{1/2}_{L^2(\mathbb{R})}\|\partial_x u\|^{1/2}_{L^2(\mathbb{R})}\|u\|_{L^2(\mathbb{R})}$$

or, equivalently,

$$\|\partial_x u\|^{3/2}_{L^2(\mathbb{R})} \leq \|\partial_x^3 u\|^{1/2}_{L^2(\mathbb{R})}\|u\|_{L^2(\mathbb{R})}\,.$$

Thus,

$$\|\partial_x u\|_{L^2(\mathbb{R})} \leq \|\partial_x^3 u\|^{1/3}_{L^2(\mathbb{R})}\|u\|^{2/3}_{L^2(\mathbb{R})}$$

and so Young's inequality gives

$$\|\partial_x u\|_{L^2(\mathbb{R})} \leq \varepsilon\|\partial_x^3 u\|_{L^2(\mathbb{R})} + C(\varepsilon)\|u\|_{L^2(\mathbb{R})}\,,$$

for any given ε and a constant $C(\varepsilon)$. We choose $\varepsilon = 1/\big(12\|\phi_0(t)\|_{L^\infty(\mathbb{R})}\big)$ so that

$$\|6\phi_0(t)\partial_x u + ku\|_{L^2(\mathbb{R})} \leq \frac{1}{2}\|\partial_x^3 u\|_{L^2(\mathbb{R})} + C\|u\|_{L^2(\mathbb{R})}\,,$$

which fulfills the relative boundedness condition (3.21). The required result now follows.

Hypothesis 2 is also fulfilled by virtue of the above argument. To prove hypothesis 3, we define a derivative operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(A(t)\upsilon\big) := -6\partial_x\upsilon\frac{\mathrm{d}}{\mathrm{d}t}\phi_0(t) - 6\upsilon\frac{\mathrm{d}}{\mathrm{d}t}(\partial_x\phi_0(t))$$

for the mapping $t \mapsto A(t)\upsilon$, for $\upsilon \in H^3(\mathbb{R})$. It is then straightforward to check that

$$\begin{aligned}\Big\|A(t)\upsilon - A(t_0)\upsilon - \frac{\mathrm{d}}{\mathrm{d}t}\big(A(t)\upsilon\big)(t-t_0)\Big\|_{L^2(\mathbb{R})} \\ \leq \|6\partial_x\upsilon\big(\phi_0(t) - \phi_0(t_0) - (\mathrm{d}/\mathrm{d}t)\phi_0(t_0)(t-t_0)\big)\|_{L^2(\mathbb{R})} \\ + \|6\upsilon\big(\partial_x\phi_0(t) - \partial_x\phi_0(t_0) - (\mathrm{d}/\mathrm{d}t)(\partial_x\phi_0(t_0))(t-t_0)\big)\|_{L^2(\mathbb{R})}\,.\end{aligned} \tag{3.22}$$

Since $\phi_0(t)$ and $\partial_x\phi_0(t) \in C^\infty\big([0,T];L^2(\mathbb{R})\big)$ it follows (using the fact that both υ and $\partial_x\upsilon \in H^1(\mathbb{R})$ and therefore $\in L^\infty(\mathbb{R})$) that the right-hand-side of (3.22) is $o(|t-t_0|)$, as required. The final hypothesis is fulfilled as a result of known properties of the KdV bisoliton.

Hence, (3.13) has a unique classical solution, as indicated in Theorem 3.7. It should be remembered, however, that one would like to have existence of a solution over *infinite* time, in keeping with our expectations of a correcting equation for KdV. Despite considerable effort in this direction it has not been possible to establish such a long-time existence result for (3.13) - i.e. persistence of solutions in the limit $\kappa \to \infty$ has not been demonstrated. Nevertheless, the finite-time result which we *do* have is sufficient to justify numerical simulation of the problem. This is the subject of the next Section.

3.4 Recasting of the problem

Now that we have both the form of the lattice corrections to 'steady state' solitons (Chapter 2) and an equation governing how these corrections evolve along the lattice (equation (3.11)), it should be possible to observe how *two* such corrections interact. This is, of course, only possible if there are two interacting solitons on the lattice. This situation can achieved by looking at bisoliton solutions to KdV.

The programme is as follows: take the pair of equations defined for $x \in (-\infty, \infty)$

$$\partial_x^3 u + 6u\,\partial_x u + \partial_t u = 0\,, \tag{3.23}$$

$$\partial_x^3 v + 6\partial_x(\phi_0 v) + \partial_t v = \frac{1}{2\alpha\beta}(\beta^2 - 2\alpha\gamma)\partial_x(\phi_0^3) - \frac{\beta}{2\alpha}\phi_0\partial_x^3\phi_0 - \frac{\beta}{40\alpha}\partial_x^5\phi_0 - \frac{9\beta}{8\alpha}\partial_x\big((\partial_x\phi_0)^2\big)\,, \tag{3.24}$$

where ϕ_0 in (3.24) is a bisoliton solution to (3.23) under the boundary conditions $u \to 0$ as $|x| \to \pm\infty$. We similarly take $v \to 0$ as $|x| \to \pm\infty$ as our boundary conditions on (3.24). Our objective is to solve (3.24), subject to suitable initial conditions, over the time period during which the two single solitons in ϕ_0 interact/collide.[1] As already discussed, the initial data should be given at $t = -\infty$ as the sum of two corrections to two dissociated single solitons (see final paragraph of Section 3.2 and equation (3.12)). Although (3.12) gives the 'right idea' as regards the type of initial data needed, it is, as we shall see, not entirely accurate.

Therefore, before describing in detail the numerical scheme used, we take a 'side-step' to describe how (3.24) can be used to derive a more general form of (2.11). This form will prove vital when stipulating the correct initial data.

The derivation is essentially the same as the recovery of (2.11) from (3.11), described in the latter part of Section 3.2. The difference here is that we shall allow the wavespeed to be an *unspecified* number. We proceed as follows:

1. make the travelling wave ansatz $\eta = x - 4a^2t$ in both equations (3.23) and (3.24), to obtain a single soliton solution $s_a = 2a^2\mathrm{sech}^2(a(\eta - \delta))$ (for any fixed constant δ) in the first case and an ODE

$$\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}v + 6\phi_0 v - 4a^2 v = \Big(\frac{\beta}{\alpha} - \frac{\gamma}{\beta}\Big)\,\phi_0^3 - \frac{\beta}{\alpha}a^2\phi_0^2 - \frac{\beta}{40\alpha}\frac{\mathrm{d}^4}{\mathrm{d}\eta^4}\phi_0 - \frac{9\beta}{8\alpha}\Big(\frac{\mathrm{d}}{\mathrm{d}\eta}\phi_0\Big)^2$$

   in the second case;

2. put $\phi_0 = s_a$ to obtain, after some simplification, the 'general wavespeed' version

[1] We follow standard nomenclature in specifying that, away from interaction, a bisoliton is composed of two single solitons. These single solitons are different from (although asymptotically equivalent to) truly independent "free" solitons. The latter will be referred to as 'dissociated single solitons'.

of $(2.11)^2$

$$\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}v + 4a^2\big(3\mathrm{sech}^2(a(\eta-\delta)) - 1\big)v = 8a^6\left(\frac{3\beta}{\alpha} - \frac{\gamma}{\beta}\right)\mathrm{sech}^6(a(\eta-\delta)) - 16a^6\,\frac{\beta}{\alpha}\,\mathrm{sech}^4(a(\eta-\delta)) - a^6\,\frac{4\beta}{5\alpha}\,\mathrm{sech}^2(a(\eta-\delta))\,; \tag{3.25}$$

3. solve (3.25) subject to zero boundary conditions to give a solution, which we denote by c_a, representing the accurate lattice correction to s_a.

Figures 3.1 and 3.2 show two pictures of s_a with corresponding c_a for two different values of a. The potential chosen in both cases is Lennard-Jones. It is worth pointing out that, in contrast with the 'steady state' case (see page 32), there is no linear correspondence between the soliton's amplitude and that of its correction. In particular, the correction's amplitude grows faster with a than does the soliton's. This is intriguing as it implies that the lattice imposes an over-proportional correction upon faster moving waves.

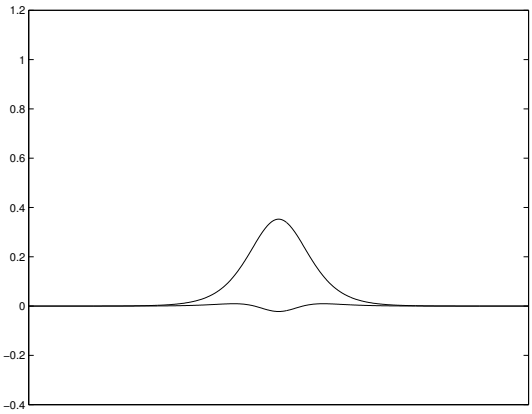


Figure 3.1: Dissociated soliton with $a = 0.42$ and corresponding correction.

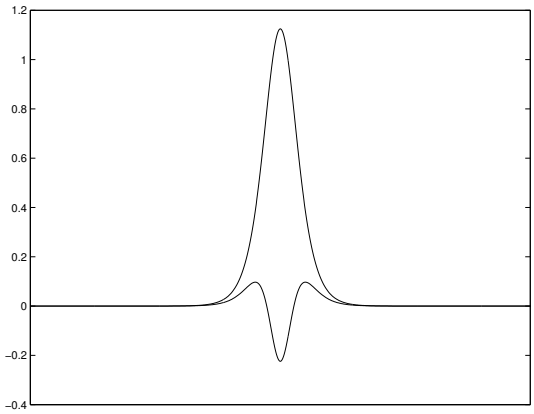


Figure 3.2: Dissociated soliton with $a = 0.75$ and corresponding correction.

However, since the correction is not necessarily single signed (as is the case in Figures 3.1 and 3.2) this may at first appear to contradict a result from [FP99]. The result in question ([FP99], Proposition 7.1) states that the lattice solitons (i.e. the solitary wave solutions to the full lattice equations) have monotonic fall off, thus

[2]Note that (3.25) will not reduce to (2.11) on substitution of $a = (\alpha/8\beta)^{1/2}$ since η is a different ansatz from θ of Section 3.2. Basically, (3.25) is a "stretched coordinate" version of (2.11).

implying that they can have only one critical point. If the wavespeed a is too great, however, the rate of growth of the correction's profile compared to that of the soliton will result in the sum $s_a + \varepsilon^2 c_a$ tending to adopt ever more closely the double-maxima profile of c_a. This would imply that the lattice soliton is in fact closer in shape to the correction than it is to the soliton at high speeds, and this is a contradiction.

The solution to this anomaly is to note that the lattice speed under consideration in [FP99] is $c = \sqrt{\alpha}\big(1 + (\varepsilon^2/24)\,\mu\big)$, where μ is fixed a priori. It is then stated that whenever c is sufficiently close to $\sqrt{\alpha}$, the monotonic fall off result holds. In other words, $(\varepsilon^2/24)\,\mu$ must be sufficiently close to zero. Thus, ε depends upon μ. Our equation (3.25) is, in essence, just (2.11) obtained by setting $\mu = a$ rather than $\mu = 1$ - the implicit value of μ in (2.11) (see (2.7)). By changing a without giving consideration to the implied threshold for ε, we run the risk of distancing c from $\sqrt{\alpha}$ by too great an extent. Moreover, we invalidate the foregoing "small ε" arguments of Chapter 2. In fact, this could well be the case even if $s_a + \varepsilon^2 c_a$ *does* display monotonic fall off.

We take from this discussion that it is acceptable to vary a only as long as we vary ε inversely, thus ensuring that we remain within our chosen regime. In the case of two solitons with differing wavespeeds, we choose ε sufficiently small to keep the faster of the two solitons within the correct regime. The same will then automatically be true of the slower soliton. Despite this, the numerical results presented in Section 3.6 will occasionally be displayed with $\varepsilon = 1$. This should not be taken to mean that $\varepsilon = 1$ is within the allowed threshold, but rather that smaller values of ε would have made the display uninformative. In all cases, however, the combination of the a and ε values will, at the very minimum, ensure that $s_a + \varepsilon^2 c_a$ has only monotonic fall off.

The first use we make of (3.25) is as part of a 'consistency check' on (3.24). Specifically, we intend to verify that the travelling wave solution of (3.25) solves (3.24) for all x and t. Since x coincides with η at $t = 0$, it should be possible to take the solution of (3.25) (for some fixed a) and use it as the $t = 0$ initial data for (3.24). We may adjust the position of the initial condition on the real line by changing δ. We then solve (3.24) over some period of time and we expect to witness the unchanging translation of the initial condition over this time. The stability of our numerical code will be tested against how well it fulfills this criterion.

We now return to the problem of interacting lattice solitons. The explicit bisoliton solution (for example [MH86] and [Hir71]) reveals that far away from the interaction time, the two solitons which make up the bisoliton appear very much like single 'dissociated' solitons. Indeed at $t = -\infty$ the bisoliton is given exactly as the sum

of two dissociated solitons. Our simulation is started sufficiently far back in time to ensure that the two soliton parts of the bisoliton solution are in effect dissociated. (3.25) will now be of use because the initial data can be given (as suggested by (3.12)) as the sum of two corrections to two single solitons. Note that since each of the two solitons will have different wavespeeds, a different value of a must be taken in obtaining, from (3.25), each of the two corrections. This will lead to the initial data being the sum of two differently shaped dissociated single soliton corrections. We now see why (3.12) is not entirely accurate: the two functions ϕ_{CORR} will *not* be identical.

Thus, given the two dissociated solitons s_{a_1} and s_{a_2} with wavespeeds a_1 and a_2 respectively, which make up the bisoliton solution to (3.23) at $t = -\infty$, we have the appropriate initial data c_{a_1} and c_{a_2}, obtained using (3.25). We are now almost ready to solve (3.24) numerically with ϕ_0 taken to be a bisoliton solution to (3.23) such that the dissociated wavespeeds of its two solitons are a_1 and a_2, respectively.

We make one final technical remark: although the simulation is notionally started at $t = -\infty$, it is in practice started at $t = 0$ where the argument of the solution of (3.25) coincides with x. The corrections can be positioned to mimic asymptotic separation by the choice of δ.

The problem to be solved numerically may now be posed thus:

$$\partial_x^3 v + 6\partial_x(\phi_0 v) + \partial_t v = \frac{1}{2\alpha\beta}(\beta^2 - 2\alpha\gamma)\partial_x(\phi_0^3) - \frac{\beta}{2\alpha}\phi_0\partial_x^3\phi_0 - \frac{\beta}{40\alpha}\partial_x^5\phi_0 - \frac{9\beta}{8\alpha}\partial_x\big((\partial_x\phi_0)^2\big)\,, \tag{3.26}$$

where ϕ_0 denotes a bisoliton solution to KdV with specified asymptotic wavespeeds a_1 and a_2, subject to

$$v|_{t=0} = \phi^{(1)}_{\mathrm{CORR}} + \phi^{(2)}_{\mathrm{CORR}}\,, \tag{3.27}$$

where $\phi^{(i)}_{\mathrm{CORR}}$ denote solutions of (3.25) with $a = a_i$ and $\delta = \delta_i$. We specify that δ_i be chosen such that they are equal to the corresponding parameters in ϕ_0.[3] By "corresponding parameters" we mean the solitons' shifts backwards along the lattice induced by tending $t \to -\infty$. Apart from an important dependence upon the ratio of $(a_1 - a_2)$ to $(a_1 + a_2)$, these shifts are $4a_1^2t$ and $4a_2^2t$. We require that the chosen t be so negative that the solitons in ϕ_0 are indistinguishable from dissociated solitons.

[3]To this end, it is easier, as indicated by the form of (3.12), to replace δ_2 by $\delta_2 + (1/2)\ln A$ (where $A = \big((a_1 - a_2)/(a_1 + a_2)\big)^2$). δ_2 should then be equated to the corresponding ϕ_0 parameter value, which will be $4a_2^2t$.

3.5 The numerical code

We now discuss the numerical scheme used to solve (3.26).[4] The scheme is based around an extension to the method proposed in [RM67] for solving the following 'tri-diagonal' problem:

$$-A_i u_{i+1} + B_i u_i - C_i u_{i-1} = d_i\,, \quad 0 \leq i \leq N \tag{3.28}$$

with $u_0 = au_1 + b$ and $u_N = c$ as boundary conditions on u. A_i, B_i, C_i and d_i are the i^{th} elements of vectors of real numbers. The method is a recurrence relation of the form

$$u_i = E_i u_{i+1} + f_i \tag{3.29}$$

which, along with knowledge of the boundary condition $u_N = c$, allows the computation of every u_i. The coefficients E_i and f_i in (3.29) can be found in terms of A, B, C, d, E_{i-1} and f_{i-1} by substituting (3.29) into (3.28) and then equating coefficients with (3.29). Given that $E_0 = a$ and $f_0 = b$, we are then able to compute all coefficients E_i and f_i.

The extension to this method which will be used here to solve (3.26) was employed successfully in [KMI77] to solve a very similar problem within the field of ion-acoustic waves (see page 37). Letting $v_i^j := v(ih, j\Delta t)$ for some small numbers h and Δt and for $0 \leq i, j \leq N$, we can write (using standard superscript/subscript discrete notation) the central-difference approximation to (3.26) as

$$\frac{1}{\Delta t}\big(v_i^{j+1} - v_i^j\big) + \frac{3}{h}\big(v_{i+1}^{j+1} - v_{i-1}^{j+1}\big)\big(\phi_0\big)_i^j + 6v_i^{j+1}\big(\partial_x\phi_0\big)_i^j \\ + \frac{1}{2h^3}\big(v_{i+2}^{j+1} - 2v_{i+1}^{j+1} + 2v_{i-1}^{j+1} - v_{i-2}^{j+1}\big) = \big(S(\phi_0)\big)_i^j\,,$$

where $S(\phi_0)$ denotes the right-hand-side of (3.26). This may be re-arranged into the following form:

$$A\, v_{i+2}^{j+1} + B_i^j\, v_{i+1}^{j+1} + C_i^j\, v_i^{j+1} - B_i^j\, v_{i-1}^{j+1} - A\, v_{i-2}^{j+1} = d_i^j \tag{3.30}$$

where

$$A = \frac{\Delta t}{2h^3}\,,\ B_i^j = \Big(\frac{3\Delta t}{h}\big(\phi_0\big)_i^j - \frac{\Delta t}{h^3}\Big)\,,\ C_i^j = \Big(1 + 6\Delta t\big(\partial_x\phi_0\big)_i^j\Big)\,,\ d_i^j = v_i^j + \Delta t\big(S(\phi_0)\big)_i^j\,.$$

(3.30) can be viewed as the more general 'penta-diagonal' version of (3.28). The boundary condition $v_{N+1}^{j+1} = v_{N+2}^{j+1} = 0$ is imposed. The 'bottom end' boundary

[4] The full code, written in MATLAB, is stored at mcmillan.maths.ox.ac.uk and may be supplied on request.

condition, required in the tri-diagonal case to allow computation of the coefficients E_i and f_i, will be replaced below by a constraint on the coefficients themselves. We now require to find the corresponding version of (3.29). This shall be of the form

$$v_i^{j+1} = E_i^j \, v_{i+2}^{j+1} + F_i^j \, v_{i+1}^{j+1} + g_i^j \, . \tag{3.31}$$

By the process of substitution and equation of coefficients outlined in the tri-diagonal case, it is possible to obtain suitable recurrence relations for E, F and g:

$$E_i^j = -\frac{A}{r_i^j} \, , \; F_i^j = \frac{1}{r_i^j}\big(-B_i^j + E_{i-1}^j (A F_{i-2}^j + B_i^j)\big) \, , \; g_i^j = \frac{1}{r_i^j}\big(d_i^j + g_{i-1}^j (A F_{i-2}^j + B_i^j) + A g_{i-2}^j\big) \, ,$$

$$r_i^j = C_i^j - A E_{i-2}^j - F_{i-1}^j (A F_{i-2}^j + B_i^j) \, , \quad \text{for} \quad 3 \leq i \leq N \tag{3.32}$$

Note the decoupling of time dependence between the relations in (3.32) as compared with (3.31). This allows (3.31) to be solved in a step-by-step manner, with the coefficients (3.32) (or, more precisely, the coefficient g_i^j - the only coefficient to depend upon v_i^j) being recalculated at each step. We take $E_{-1}^j = F_{-1}^j = g_{-1}^j = E_0^j = F_0^j = g_0^j = 0$, which is means setting

$$E_1^j = -\frac{A}{C_1^j} \, , \quad F_1^j = -\frac{B_1^j}{C_1^j} \, , \quad g_1^j = \frac{d_1^j}{C_1^j}$$

and

$$E_2^j = -\frac{A}{C_2^j - B_2^j \, F_1^j} \, , \quad F_2^j = \frac{-B_2^j + E_1^j \, B_2^j}{C_2^j - B_2^j \, F_1^j} \, , \quad g_2^j = \frac{d_2^j + g_1^j \, B_2^j}{C_2^j - B_2^j \, F_1^j} \, .$$

Although other numerical schemes (discussed below in Section 3.7) may also be successful in solving third order equations of the type to which (3.26) belongs, the scheme described in this Section was ultimately chosen due to its simplicity and our ability to cross-check its performance against the results in [KMI77]. The results obtained are presented in the following Section.

3.6 Numerical results

The code outlined in the previous Section was tested first by reproducing the results of [KMI77]. This was done with little difficulty. A greater challenge was posed by our own equation (3.26) which differs from the corresponding equation studied in [KMI77] by its inclusion of a term within $S(\phi_0)$ which is third order in ϕ_0. The parameters in (3.26) were set as follows:

$$\alpha = 1 \, , \quad \beta = 1 \, , \quad \gamma = 53/63 \, ,$$

which means we are looking here exclusively at the Lennard-Jones case.[5]

The first test of the code on equation (3.26) was for the case of the single soliton - i.e. the simple evolution of the travelling wave in the absence of collision. Details of this case were outlined on page 47. The objective was to achieve as little distortion as possible over the time period of interest. Figure 3.3 shows the result of running the evolution over a period of 10 time units with a temporal mesh discretization of 1/512 and spatial mesh discretization of approximately 1/625. a was taken equal to 0.75. Figure 3.3 shows only the central portion (30 units approximately) of the whole space (65 units) over which the computation was done. The reason for the large sections of empty space on either side of the evolving correction is to avoid interference with the boundaries, which is known to be particularly damaging to the simulation of third order differential operators.

The discretization accuracy required for the computation necessitated the use of a large-memory computer. After having loaded the variables in their correct form onto the workspace, the computations in this Section required around 1 hour to complete. This gives an indication that the evolution equation we are simulating may be "stiff".

Figures 3.4 and 3.5 provide a clearer view of the distortion experienced by the correction profile during the evolution. Although some distortion has taken place, the result was judged sufficiently successful to allow us to proceed, with this level of accuracy and over this time interval, to the simulation of the collision process.

Another measure of the stability of the code is the extent to which the total mass $\int_{-\infty}^{\infty} v$ is preserved. See Section 3.7 for details of why this should be the case. It was found that the total mass increased by 30% between Figure 3.4 and Figure 3.5. This was the lowest mass change obtainable with the hardware at our disposal. Although this is a significant change, it was found, by careful examination, that mass growth of this type was *not* a significant factor in our ability to accurately model the collision process. Distortion of the profile was a much more important concern.

[5]Our ability to repeat the ensuing numerical calculations with other potentials was limited due to serious computer capacity constraints.

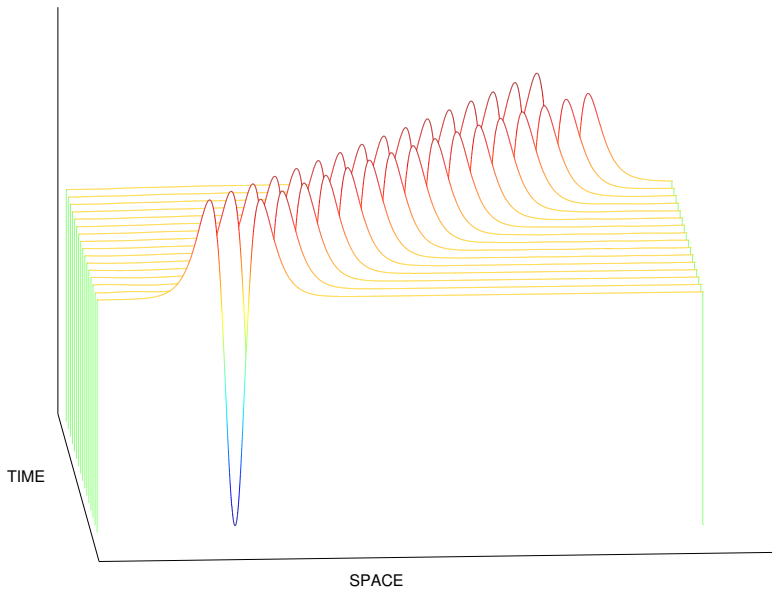


Figure 3.3: The evolution of the single soliton correction.

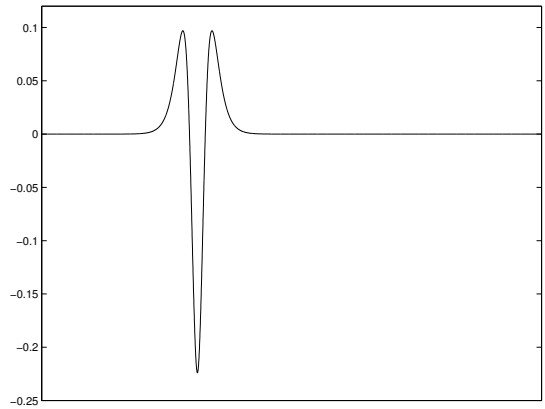


Figure 3.4: The initial data for the evolution of the single soliton correction.

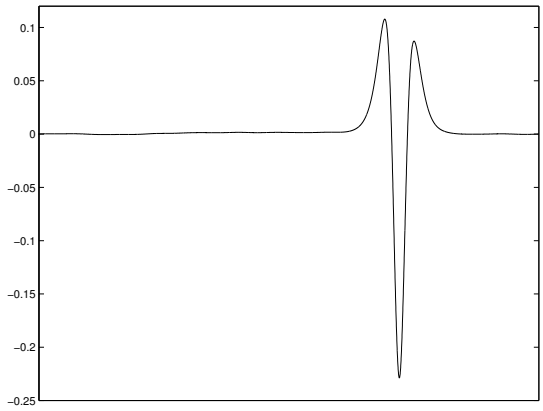


Figure 3.5: The final profile of the single soliton correction.

We now present the results of the collision simulation. Figure 3.6 and Figure 3.7 show that the collision process has a profound effect upon the corrections' profiles. From the point of view of stability of the code during this evolution, it is encouraging to note the stabilization of the profiles of the corrections *after* collision.

Figures 3.8 and 3.9 show the extent of the impact of collision upon the correction profiles. Both the slow and the fast corrections become asymmetric. The leading section of the fast correction becomes entirely positive and the trailing section becomes entirely negative. The opposite is true of the slower correction. The mass growth between Figure 3.8 and 3.9 is around 17%.

The loss of symmetry, as seen in Figure 3.7 in particular, indicates that the effect of the corrections upon the solitons is, after collision, to permanently shift forward the fast soliton and shift backward the slow soliton, compared with their uncorrected positions. This surprising effect is illustrated specifically in Figure 3.10.

Figure 3.10 consists of an uncorrected bisoliton and a corrected bisoliton. The correction was added with a prefactor of $\varepsilon = 1$. The impact of the correction after collision is most clearly visible for the fast soliton, where the corrected soliton is shifted forwards relative to its uncorrected counterpart.

The correction thus affects the bisoliton by creating an effective repulsion between the post-collision solitons. The behaviour is contrary to that seen in [KMI77] for ion-acoustic waves. In that case, the bisoliton correction was found to give rise to an effective *attraction* between the post-collision solitons.

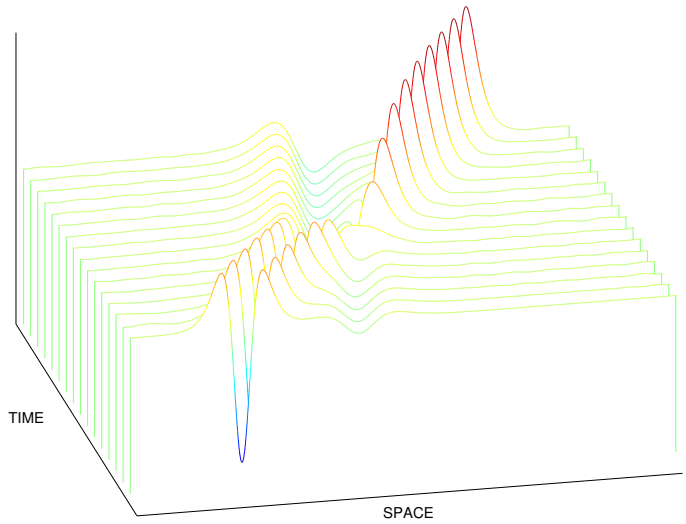


Figure 3.6: An elevation view of the collision of the bisoliton correction.

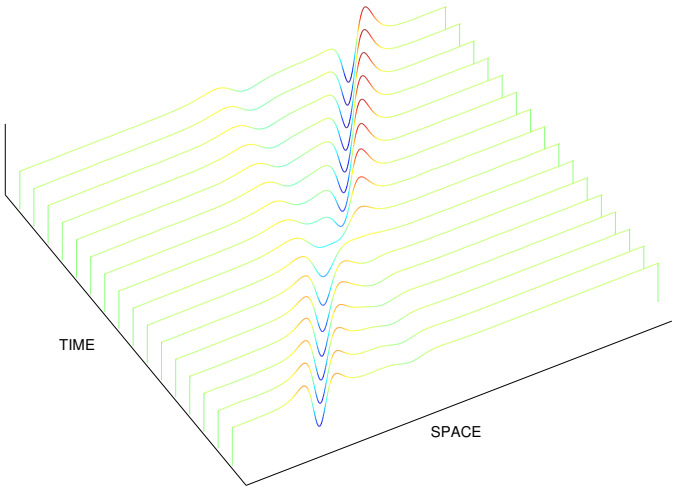


Figure 3.7: An overhead view of the collision of the bisoliton correction.

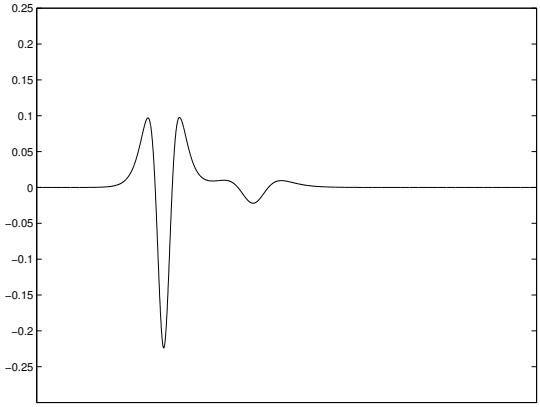


Figure 3.8: The initial data for the collision of the bisoliton correction.

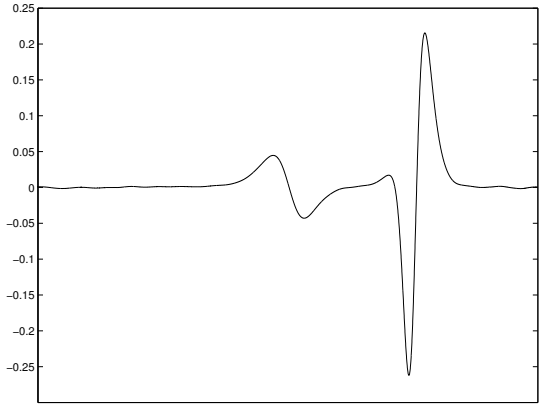


Figure 3.9: The final profile of the bisoliton correction after collision.

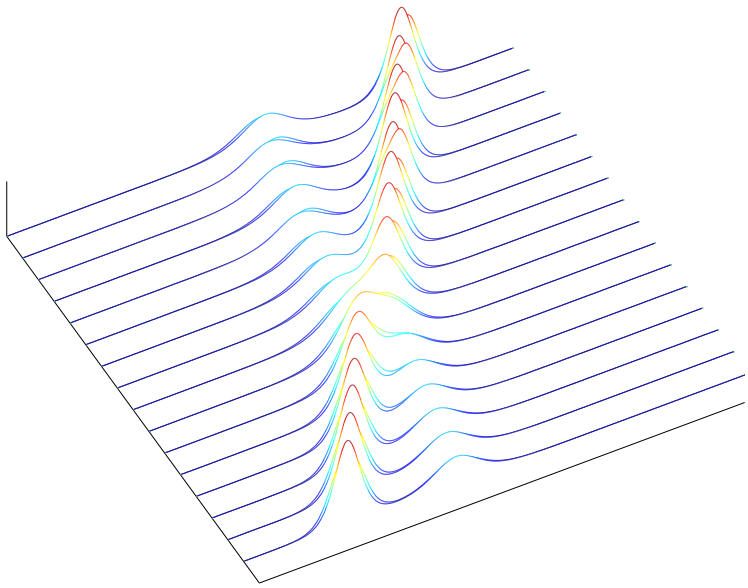


Figure 3.10: The collision of the corrected and uncorrected bisoliton.

3.7 Discussion of alternative schemes

In this penultimate Section, we look at other ways in which we might have numerically simulated our correcting equation (3.11). We shall focus particularly upon symplectic methods and shall discuss the theory behind such 'volume preserving' techniques.

We begin by showing that, as promised earlier, *mass* is a conserved quantity for equation (3.11). We go on to observe that (3.11) may be rewritten in Hamiltonian form, thus establishing the existence of a conserved *energy* functional. The existence of this Hamiltonian representation then justifies our discussion of numerical symplectic methods.

Conservation of mass is proven by observing that (3.11) may be rearranged so that $\partial_t \phi_1$ is equated to the sum of an x derivative and a constant multiple of $\phi_0 \partial_x^3 \phi_0$. Taking the integral with respect to x of $\partial_t \phi_1$ between $-\infty$ and ∞ we obtain

$$\partial_t \int_{-\infty}^{\infty} \phi_1 = -\frac{\beta}{2\alpha} \int_{-\infty}^{\infty} \phi_0 \partial_x^3 \phi_0 \,, \tag{3.33}$$

by using appropriate zero boundary conditions for ϕ_1 and its x derivatives and by using the decay of ϕ_0 and its x derivatives at $\pm\infty$. Two integrations by parts of the right-hand-side of (3.33) give

$$\int_{-\infty}^{\infty} \phi_0 \partial_x^3 \phi_0 = -\int_{-\infty}^{\infty} \partial_x \phi_0 \partial_x^2 \phi_0 = \int_{-\infty}^{\infty} \partial_x^2 \phi_0 \partial_x \phi_0 \,,$$

thus proving that the $\partial_t \int_{-\infty}^{\infty} \phi_1 = 0$, as required.

A Hamiltonian representation for (3.11) is achieved (if we change notation from ϕ_1 to u) by rewriting the equation as

$$\frac{\partial u}{\partial t} = \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial H}{\partial u} \,, \tag{3.34}$$

where

$$H(u) := \int \Big(\frac{1}{2} u_x^2 - 3\phi_0 u^2 + F \Big) \, \mathrm{d}x \,,$$

and $\partial H / \partial u$ denotes the Fréchet derivative of H with respect to the standard scalar product on $L^2(\mathbb{R})$. ϕ_0 denotes a multi-soliton solution of KdV, expressible in the form of the right-hand-side of (3.8), and F is the integral from $-\infty$ to x of the right-hand-side of (3.11). Explicitly,

$$F := \frac{1}{2\alpha\beta}(\beta^2 - 2\alpha\gamma)\phi_0^3 - \frac{\beta}{2\alpha}\tilde{\Phi}_0 - \frac{\beta}{40\alpha}\partial_x^4 \phi_0 - \frac{9\beta}{8\alpha}(\partial_x \phi_0)^2 \,,$$

where $\tilde{\Phi}_0 := \int_{-\infty}^{x} \phi_0 \partial_x^3 \phi_0 \mathrm{d}x$. Equivalently, $\tilde{\Phi}_0$ may be expressed as

$$\tilde{\Phi}_0 = \phi_0 \partial_x^2 \phi_0 - \frac{1}{2}(\partial_x \phi_0)^2 \,,$$

so that

$$F = \frac{1}{2\alpha\beta}(\beta^2 - 2\alpha\gamma)\phi_0^3 - \frac{\beta}{2\alpha}\phi_0 \partial_x^2 \phi_0 - \frac{\beta}{40\alpha}\partial_x^4 \phi_0 - \frac{7\beta}{8\alpha}(\partial_x \phi_0)^2 \,.$$

Hence, (3.11) possesses the structure of an infinite dimensional Hamiltonian system and may therefore be thought of as symplectic in that sense.

Following [SSC94], we are able to conceive of numerical schemes which conserve the symplectic nature of ordinary differential equations (in finite dimensions). Among these are the class of symplectic Runge-Kutta methods. It is possible to exploit these techniques when numerically solving (3.11). We begin by defining $U := \mathcal{F}^{-1}(e^{-i\xi^3 t}\widehat{\phi_1})$. Then, (3.11) may be written

$$\widehat{U}_t = -6i\xi e^{-i\xi^3 t}\widehat{\phi_0 \phi_1} + e^{-i\xi^3 t}\widehat{f} \,, \tag{3.35}$$

where f denotes the right-hand-side of (3.11). (3.35) may now be written solely in terms of U as follows:

$$\widehat{U}_t = -6i\xi e^{-i\xi^3 t}\mathcal{F}\big(\phi_0 \mathcal{F}^{-1}(e^{i\xi^3 t}\widehat{U})\big) + e^{-i\xi^3 t}\widehat{f} \,. \tag{3.36}$$

If we now discretise in the ξ direction we obtain a system of ODEs of the form

$$V_t = K(V, t) \,, \tag{3.37}$$

for some known function K. It is therefore possible to discretise and solve (3.36) via a symplectic Runge-Kutta method.[6] Having done this, ϕ_1 is easily recovered. We have, in effect, removed the x derivatives from (3.11) by the use of a standard spectral technique (see, for example, [Tre00]).

If we define $V^n := \widehat{U}(\xi, n\Delta t)$ and $t = n\Delta t$, the (s stage) Runge-Kutta method which could be used for (3.36) viewed in form (3.37) may be written down as follows:

$$V^{n+1} = V^n + \Delta t \sum_{i=1}^{s} b_i K(Y_i, t + c_i \Delta t) \,, \tag{3.38}$$

[6]It is of interest to note, in relation to Fourier transforms of Hamiltonian systems, that a result by Wang [Wan91] ensures that, for appropriate initial data, it is possible to replace an infinite dimensional system of the form (3.34) by a finite dimensional system in terms of only a finite number of Fourier coefficients such that (under reasonably broad conditions) the finite system preserves either many or all of the infinite system's conservation laws. Although it does not follow immediately that the same is true of the discretisation of (3.36), there is nevertheless a strong indication from [Wan91] that this should be case. Our own approach is favoured here only due to its simplicity.

where, for $i = 1, \ldots, s$,

$$Y_i = V^n + \Delta t \sum_{j=1}^{s} a_{ij} K(Y_j, t + c_j \Delta t)\,, \tag{3.39}$$

$$c_i = \sum_{j=1}^{s} a_{ij}\,.$$

We are free to choose the numbers a_{ij} and b_i as we wish and we note that if $a_{ij} = 0$ whenever $i \leq j$, then (3.39) is in fact a recurrence relation for the 'stages' Y_i in terms of the preceding Y_l, $l < i$. The scheme is then said to be *explicit*.

If a_{ij} and b_i are chosen such that

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0\,, \quad i, j = 1, \ldots, s\,,$$

then by Theorem 6.1 of [SSC94], the method will be symplectic, in the sense that the (notional) time stepping operator $\Psi(t, t + \Delta t) : V^n \mapsto V^{n+1}$ is a symplectic transformation. By setting $i = j$ we see that such a method cannot be explicit. It is always *implicit*. In addition, as noted in [SSV89], many implicit Runge-Kutta methods have the advantage of preserving the 'contractive' nature of solutions.[7] Contractivity is a property possessed, for example, by dissipative systems (i.e. systems where the spatial differential operator is dissipative) and if preserved by the numerical approximation it can prove valuable in overcoming the difficulties encountered if the system happens to be "stiff".

As an example of a symplectic choice of a_{ij} and b_i we have

$$a_{11} = a_{22} = \frac{1}{4}\,, \quad a_{12} = \frac{1}{4} - \frac{\sqrt{3}}{6}\,, \quad a_{21} = \frac{1}{4} + \frac{\sqrt{3}}{6}\,, \quad b_1 = b_2 = \frac{1}{2}\,.$$

This method is commonly known as the two-stage Gauss method. All Gauss methods are particularly note-worthy because they are 'optimal' in the sense that the order of the error induced by stepping from one time-step to another (as compared with the true solution) is as high as possible for any time-stepping method.

We have therefore seen some of the advantages which could be had from using alternative numerical schemes for solving (3.11). These may offer a good way of verifying the results of Section 3.6. It should be noted, however, that by no means all numerical schemes will successfully solve (3.11). For example, it was found that an *explicit* (i.e. non-symplectic) 4^{th} order Runge-Kutta method is unable to solve (3.11) to any useful degree of accuracy.

[7] Contractivity refers to the tendency among solutions to certain PDEs generated from different initial data to approach one another as time progresses. Solutions of the heat equation possess this property.

3.8 Concluding remarks

In this Chapter we have formally derived an evolution equation for discreteness effects on the generic FPU lattice. We have shown that this equation is consistent with the rigorously justified 'steady state' equation discussed in Chapter 2. We have proved that the evolution equation possesses a unique (finite time) solution and have been able to write down the relevant initial conditions for the physical problem which we wish to consider. In the last two Sections we examined how the equation may be numerically simulated. Realising that the equation was already known in both the fields of shallow water wave theory and ion-acoustic wave theory, we were able to adapt a numerical scheme which had already been successfully used on a very similar equation [KMI77]. Although we were able to replicate the results of [KMI77], we found that a numerically stable simulation of our own equation required extensive computing power and a large amount of computing time.

Nevertheless, we *were* able to produce qualitatively valid results for the collision of two lattice solitons. This revealed that the discreteness of the lattice tends to produce an effective 'repulsive' interaction between two post-collision lattice solitons (as compared with exact continuum solitons). This was unexpected behaviour and was also contrary to the 'attractive' interaction exhibited by colliding ion-acoustic waves. In particular, the predicted lattice radiation was *not* visible. However, the repulsive interaction may itself be interpreted as the emergence of an expansive phenomenon in the lattice between two post-collision solitons. Although this is not sufficient to infer the existence of lattice radiation, it does indicate that lattice discreteness has a profound impact upon colliding solitons.

The most likely explanation for the absence of the radiation predicted in [FPP89] and [Lee] from our results, is simply that the long-wave regime is not the correct one for direct visualisation of this phenomenon. It is likely that something close to the inversion of the fully discrete lattice operator would be required in order to reveal the radiative term.

Another possible explanation, by analogy with the theory of soliton transmission in optical fibres [AA97], is that radiation is in fact a higher order effect. Radiation appears in that theory as a fourth order perturbation to the integrable nonlinear Schrödinger equation.

Finally, we mention also the question of stability of the lattice bisoliton. To our knowledge no rigorous analysis exists to address this issue. It is known that under some conditions lattice equations may become chaotic and even disordered. To

properly account for lattice radiation it may well be necessary to rule out a possible transition to chaos as a result of bisoliton interaction. (The topic of chaos in condensed matter is partially reviewed in Part 4 of [BBZ83], whereas [Abd94] deals specifically with soliton propagation across inhomogeneous media.)

In conclusion, the results put forward in this Chapter appear to be a significant contribution to the theory of nonlinear lattice equations. They help, in particular, to draw similarities between this field and the fields of shallow water wave theory and ion-acoustic theory. Many of the ideas may be carried forward by exploring whether these similarities could be further exploited or by making use of the Hamiltonian structure which underlies much of the work in this area.

Appendix A

Technical Results

Lemma A.1. *Suppose $F : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ and $\tilde{F}^{(\varepsilon)} : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ are Gâteaux differentiable in some neighbourhood of $\phi_0 \in H^1(\mathbb{R})$ (with derivatives being bounded linear maps) where ϕ_0 is such that $F(\phi_0) = \phi_0$. Moreover suppose that there exists $\phi^{(\varepsilon)} \in H^1(\mathbb{R})$ such that $F(\phi^{(\varepsilon)}) + \tilde{F}^{(\varepsilon)}(\phi^{(\varepsilon)}) = \phi^{(\varepsilon)}$, for all $\varepsilon > 0$ sufficiently small. Also, assume that $\tilde{F}^{(0)}(\psi) = 0$ for all $\psi \in H^1(\mathbb{R})$.*

Suppose $\varepsilon^2 \mapsto \tilde{F}^{(\varepsilon)}(\phi_0)$ is differentiable at $\varepsilon^2 = 0$ as a mapping from $\mathbb{R}$ into $H^1(\mathbb{R})$.

Define $A := I - DF(\phi_0) : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ and suppose A is invertible (with $A^{-1} : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ such that $\|A^{-1}\|_{H^1(\mathbb{R})\to H^1(\mathbb{R})} \leq C_0$).

Define $\phi_{\mathrm{cor}} \in H^1(\mathbb{R})$ by

$$\phi_{\mathrm{cor}} := A^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0)\right).$$

Choose $\delta > 0$ so small that

1. $$\|\phi - \phi_0\|_{H^1(\mathbb{R})} \leq \delta \Rightarrow \|DF(\phi) - DF(\phi_0)\|_{H^1(\mathbb{R})\to H^1(\mathbb{R})} \leq C_1\,;$$

2. $$\|\phi - \phi_0\|_{H^1(\mathbb{R})} \leq \delta \Rightarrow \|D\tilde{F}^{(\varepsilon)}(\phi)\|_{H^1(\mathbb{R})\to H^1(\mathbb{R})} \leq C_2\,;$$

where C_1 and C_2 are small enough to satisfy $C_0(C_1 + C_2) \leq \theta < 1$.

Then, for ε sufficiently small, the following estimate holds:

$$\begin{aligned}\|\phi^{(\varepsilon)} - \phi_0 - \varepsilon^2\phi_{\mathrm{cor}}\| \leq{}& \varepsilon^2 (1-\theta)^{-1} C_0 \|\phi_{\mathrm{cor}}\|_{H^1(\mathbb{R})} \cdot \\ &\cdot \sup_{\tau\in[0,1]} \|DF(\phi_0 + \tau\varepsilon^2\phi_{\mathrm{cor}}) - DF(\phi_0)\|_{H^1(\mathbb{R})\to H^1(\mathbb{R})} \\ &+ (1-\theta)^{-1} C_0 \left\|\tilde{F}^{(\varepsilon)}(\phi_0 + \varepsilon^2\phi_{\mathrm{cor}}) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0)\right\|_{H^1(\mathbb{R})}.\end{aligned} \tag{A.1}$$

Moreover, if, in fact $\varepsilon^2 \mapsto \tilde{F}^{(\varepsilon)}(\phi)$ is differentiable at $\varepsilon^2 = 0$ for all $\phi \in S$ where $S \subset H^1(\mathbb{R})$ includes the linear subspace of $H^1(\mathbb{R})$ spanned by ϕ_0 and $\phi_{\rm cor}$, then we may restate the estimate as follows:

$$\begin{aligned}\|\phi^{(\varepsilon)} - \phi_0 - \varepsilon^2\phi_{\rm cor}\| \leq \varepsilon^2 (1-\theta)^{-1} C_0 \|\phi_{\rm cor}\|_{H^1(\mathbb{R})} \cdot \\ \cdot \sup_{\tau\in[0,1]} \|DF(\phi_0 + \tau\varepsilon^2\phi_{\rm cor}) - DF(\phi_0)\|_{H^1(\mathbb{R})\to H^1(\mathbb{R})} \\ + (1-\theta)^{-1} C_0 \sup_{\phi\in\{\phi_0+\tau\phi_{\rm cor}:\tau\in[0,1]\}} \left\| \tilde{F}^{(\varepsilon)}(\phi) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi) \right\|_{H^1(\mathbb{R})} \\ + \varepsilon^2 (1-\theta)^{-1} C_0 \left\| \Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}\Big)(\phi_0 + \varepsilon^2\phi_{\rm cor}) - \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0) \right\|_{H^1(\mathbb{R})} .\end{aligned} \tag{A.2}$$

Proof. Let $y := \phi^{(\varepsilon)} - \phi_0$. Then,

$$\begin{aligned} Ay - \varepsilon^2 A\phi_{\rm cor} &= F(\phi_0 + y) - F(\phi_0) - DF(\phi_0)y + \tilde{F}^{(\varepsilon)}(\phi_0 + y) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0) \\ &= \big(F(\phi_0 + \varepsilon^2\phi_{\rm cor}) - F(\phi_0) - \varepsilon^2 DF(\phi_0)\phi_{\rm cor}\big) \\ &\quad + \big(\tilde{F}^{(\varepsilon)}(\phi_0 + \varepsilon^2\phi_{\rm cor}) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0)\big) \\ &\quad + \big(F(\phi_0 + y) - F(\phi_0) - DF(\phi_0)y + \tilde{F}^{(\varepsilon)}(\phi_0 + y)\big) \\ &\quad - \big(F(\phi_0 + \varepsilon^2\phi_{\rm cor}) - F(\phi_0) - \varepsilon^2 DF(\phi_0)\phi_{\rm cor} + \tilde{F}^{(\varepsilon)}(\phi_0 + \varepsilon^2\phi_{\rm cor})\big) . \end{aligned}$$

Hence, defining $T : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ by

$$T(\psi) := A^{-1}\big(F(\phi_0 + \psi) - F(\phi_0) - DF(\phi_0)\psi + \tilde{F}^{(\varepsilon)}(\phi_0 + \psi)\big) ,$$

we have

$$\begin{aligned} y - \varepsilon^2\phi_{\rm cor} &= A^{-1}\big(F(\phi_0 + \varepsilon^2\phi_{\rm cor}) - F(\phi_0) - \varepsilon^2 DF(\phi_0)\phi_{\rm cor}\big) \\ &\quad + A^{-1}\left(\tilde{F}^{(\varepsilon)}(\phi_0 + \varepsilon^2\phi_{\rm cor}) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0)\right) \\ &\quad + T(y) - T(\varepsilon^2\phi_{\rm cor}) . \end{aligned}$$

Suppose that $T : B_\delta(0) \to H^1(\mathbb{R})$ (where $B_\delta(0)$ denotes the ball of radius δ centred on 0 in $H^1(\mathbb{R})$) is a contraction with Lipschitz constant θ. Then,

$$\begin{aligned} \|y - \varepsilon^2\phi_{\rm cor}\| &\leq C_0 \|F(\phi_0 + \varepsilon^2\phi_{\rm cor}) - F(\phi_0) - \varepsilon^2 DF(\phi_0)\phi_{\rm cor}\|_{H^1(\mathbb{R})} \\ &\quad + C_0 \left\| \tilde{F}^{(\varepsilon)}(\phi_0 + \varepsilon^2\phi_{\rm cor}) - \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0} \tilde{F}^{(\varepsilon)}(\phi_0) \right\|_{H^1(\mathbb{R})} \\ &\quad + \theta \|y - \varepsilon^2\phi_{\rm cor}\|_{H^1(\mathbb{R})} . \end{aligned}$$

This immediately gives (A.1), and (A.2) follows easily by observing that

$$\begin{aligned}
&\Big\|\tilde{F}^{(\varepsilon)}(\phi_0+\varepsilon^2\phi_{\rm cor})-\varepsilon^2\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0}\tilde{F}^{(\varepsilon)}(\phi_0)\Big\|_{H^1(\mathbb{R})}\\
&\le\Big\|\tilde{F}^{(\varepsilon)}(\phi_0+\varepsilon^2\phi_{\rm cor})-\varepsilon^2\Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0}\tilde{F}^{(\varepsilon)}\Big)(\phi_0+\varepsilon^2\phi_{\rm cor})\Big\|_{H^1(\mathbb{R})}\\
&+\varepsilon^2\Big\|\Big(\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0}\tilde{F}^{(\varepsilon)}\Big)(\phi_0+\varepsilon^2\phi_{\rm cor})-\frac{\mathrm{d}}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon^2=0}\tilde{F}^{(\varepsilon)}(\phi_0)\Big\|_{H^1(\mathbb{R})}.
\end{aligned}$$

So, it remains to prove that T is indeed a contraction from $B_\delta(0)$ into $H^1(\mathbb{R})$. We have that

$$\|T(\psi_1)-T(\psi_2)\|\le C_0\left[\|F_2(\psi_1)-F_2(\psi_2)\|_{H^1(\mathbb{R})}+\|\tilde{F}^{(\varepsilon)}(\phi_0+\psi_1)-\tilde{F}^{(\varepsilon)}(\phi_0+\psi_2)\|_{H^1(\mathbb{R})}\right],$$

where $F_2(\psi):=F(\phi_0+\psi)-F(\phi_0)-DF(\phi_0)\psi$. Now,

$$F_2(\psi_1)-F_2(\psi_2)=\int_0^1\Big(DF\big(\phi_0+\psi_2+\tau(\psi_1-\psi_2)\big)-DF(\phi_0)\Big)\,\mathrm{d}\tau\cdot(\psi_1-\psi_2)$$

and so

$$\|F_2(\psi_1)-F_2(\psi_2)\|_{H^1(\mathbb{R})}\le C_1\|\psi_1-\psi_2\|_{H^1(\mathbb{R})}$$

(since $\|\phi_0+\psi_2+\tau(\psi_1-\psi_2)-\phi_0\|_{H^1(\mathbb{R})}=\|(1-\tau)\psi_2+\tau\psi_1\|_{H^1(\mathbb{R})}\le\delta$ and so fits the criteria for assumption 1). On the other hand,

$$\|\tilde{F}^{(\varepsilon)}(\phi_0+\psi_1)-\tilde{F}^{(\varepsilon)}(\phi_0+\psi_2)\|_{H^1(\mathbb{R})}\le C_2\|\psi_1-\psi_2\|_{H^1(\mathbb{R})},$$

by applying the Mean Value Theorem and assumption 2, the criterion $\|\phi-\phi_0\|_{H^1(\mathbb{R})}\le\delta$ which is met for every point ϕ lying on the line joining $\phi_0+\psi_1$ to $\phi_0+\psi_2$. The required result now follows. □

Lemma A.2. *If $f\in C^3(\mathbb{R};\mathbb{R})$ and $f(0)=0$ and if $\psi\in H^1(\mathbb{R})$, then the map $\psi\mapsto f(\psi)$ is Fréchet differentiable from $H^1(\mathbb{R})$ into $H^1(\mathbb{R})$.*

Proof. First, $\psi\mapsto f(\psi)$ is a mapping into $H^1(\mathbb{R})$, since $f\in C^1(\mathbb{R};\mathbb{R})$ and $f(0)=0$ (see [Bre99], p.131). Now, we are required to demonstrate the existence of a linear operator $L(\psi_0):H^1(\mathbb{R})\to H^1(\mathbb{R})$ for each $\psi_0\in H^1(\mathbb{R})$ such that

$$\frac{\Big\|f(\psi)-f(\psi_0)-L(\psi_0)(\psi-\psi_0)\Big\|_{H^1(\mathbb{R})}}{\|\psi-\psi_0\|_{H^1(\mathbb{R})}}\to 0,$$

as $\|\psi-\psi_0\|_{H^1(\mathbb{R})}\to 0$. Define such a linear operator by

$$L(\psi_0)t:=f'(\psi_0)\,t,$$

where $f' : \mathbb{R} \to \mathbb{R}$ is the real space derivative function of f and where $f'(\psi_0)$ acts on t by multiplication of real-valued functions. Note that since $\psi_0 \in H^1(\mathbb{R})$, $\psi_0 \in L^\infty(\mathbb{R})$ and so there exists M such that $\|\psi_0\|_{L^\infty} = M$ and hence f', $f'' : [-M, M] \to \mathbb{R}$. Thus, by continuity of f' and f'', we have $f'(\psi_0)$, $f''(\psi_0) \in L^\infty$. Using these facts it is straight-forward to demonstrate that $L(\psi_0)$ does indeed map $H^1(\mathbb{R})$ into $H^1(\mathbb{R})$. Since $f \in C^2$ (in particular) we have, for any s sufficiently close to s_0,

$$\left| f(s) - f(s_0) - f'(s_0)(s - s_0) \right| \leq C|s - s_o|^2 \,. \tag{A.3}$$

Similarly, since $f' \in C^2$, we have

$$\left| f'(s) - f'(s_0) - f''(s_0)(s - s_0) \right| \leq C|s - s_o|^2 \,. \tag{A.4}$$

Now,

$$\begin{aligned} \left\| f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right\|^2_{H^1(\mathbb{R})} &= \left\| f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right\|^2_{L^2(\mathbb{R})} \\ &\quad + \left\| \frac{\mathrm{d}}{\mathrm{d}x} \left[f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right] \right\|^2_{L^2(\mathbb{R})} \end{aligned}$$

and

$$\begin{aligned} &\left\| f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right\|^2_{L^2(\mathbb{R})} \\ &\qquad = \int_{\mathbb{R}} \left| f(\psi(x)) - f(\psi_0(x)) - f'(\psi_0(x))(\psi(x) - \psi_0(x)) \right|^2 \\ &\qquad \leq C \int_{\mathbb{R}} \left| \psi(x) - \psi_0(x) \right|^4 , \end{aligned}$$

using (A.3) and reducing, if necessary, the L^∞ distance between ψ and ψ_0 by reducing the H^1 distance. Hence,

$$\begin{aligned} \left\| f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right\|^2_{L^2(\mathbb{R})} &\leq C \|\psi - \psi_0\|^2_{L^\infty} \, \|\psi - \psi_0\|^2_{L^2} \\ &\leq C \|\psi - \psi_0\|^4_{H^1(\mathbb{R})} \,. \end{aligned}$$

Next,

$$\begin{aligned}
&\left\| \frac{\mathrm{d}}{\mathrm{d}x} \left[f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right] \right\|_{L^2(\mathbb{R})} \\
&\quad = \left\| f'(\psi)\psi_x - f'(\psi_0)\psi_x - f''(\psi_0)(\psi - \psi_0)(\psi_0)_x \right\|_{L^2(\mathbb{R})} \\
&\quad \leq \left\| f'(\psi)\psi_x - f'(\psi_0)\psi_x - f''(\psi_0)(\psi - \psi_0)\psi_x \right\|_{L^2(\mathbb{R})} \\
&\qquad + \left\| f''(\psi_0)(\psi - \psi_0)\psi_x - f''(\psi_0)(\psi - \psi_0)(\psi_0)_x \right\|_{L^2(\mathbb{R})} \\
&\quad \leq \|\psi_x\|_{L^2(\mathbb{R})} \left\| f'(\psi) - f'(\psi_0) - f''(\psi_0)(\psi - \psi_0) \right\|_{L^\infty} \\
&\qquad + \left\| f''(\psi_0)(\psi - \psi_0) \frac{\mathrm{d}}{\mathrm{d}x}(\psi - \psi_0) \right\|_{L^2(\mathbb{R})} \\
&\quad \leq \|\psi_x\|_{L^2(\mathbb{R})} \left\| f'(\psi) - f'(\psi_0) - f''(\psi_0)(\psi - \psi_0) \right\|_{L^\infty} \\
&\qquad + \left\| f''(\psi_0)(\psi - \psi_0) \right\|_{L^\infty} \left\| \frac{\mathrm{d}}{\mathrm{d}x}(\psi - \psi_0) \right\|_{L^2(\mathbb{R})} .
\end{aligned}$$

Using (A.4) we find

$$\begin{aligned}
\left\| \frac{\mathrm{d}}{\mathrm{d}x} \left[f(\psi) - f(\psi_0) - f'(\psi_0)(\psi - \psi_0) \right] \right\|_{L^2(\mathbb{R})} &\leq C\|\psi_x\|_{L^2(\mathbb{R})}\|\psi - \psi_0\|_{L^\infty} \\
&\quad + \left\| f''(\psi_0)(\psi - \psi_0) \right\|_{L^\infty} \|\psi - \psi_0\|_{H^1(\mathbb{R})}
\end{aligned}$$

and the result follows quickly from this.

□

Lemma A.3. *If $\psi \mapsto f(\psi)$ is Fréchet differentiable from $H^1(\mathbb{R})$ into $H^1(\mathbb{R})$ and if $\phi \in H^1(\mathbb{R})$, then the map $(\phi, \psi) \mapsto \phi^2 f(\psi)$ is also Fréchet differentiable from $H^1(\mathbb{R}) \times H^1(\mathbb{R})$ into $H^1(\mathbb{R})$.*

Proof. First, since $H^1(\mathbb{R})$ is a Banach algebra and since $f(\psi) \in H^1(\mathbb{R})$ and $\phi^2 \in H^1(\mathbb{R})$, it follows that $\phi^2\, f(\psi) \in H^1(\mathbb{R})$. Now, define the total derivative $D_{\psi,\phi} \left(\phi^2\, f(\psi) \right) : H^1(\mathbb{R}) \times H^1(\mathbb{R}) \to H^1(\mathbb{R})$ of $\phi^2\, f(\psi)$ by

$$D_{\phi,\psi} \left(\phi^2\, f(\psi) \right) (\nu, \tau) := 2\phi\nu \cdot f(\psi) + \phi^2 D_\psi f(\psi)(\tau) .$$

Then,

$$\begin{aligned}
&\Big\|\phi^2 f(\psi) - \phi_0^2 f(\psi_0) - D_{\phi,\psi}\big(\phi^2 f(\psi)\big)\Big|_{(\phi,\psi)=(\phi_0,\psi_0)}\big((\phi-\phi_0),(\psi-\psi_0)\big)\Big\|_{H^1(\mathbb{R})}\\
&= \Big\|\phi^2 f(\psi) - \phi_0^2 f(\psi_0) - \big[2\phi_0(\phi-\phi_0)\cdot f(\psi_0) + \phi_0^2 D_\psi f(\psi_0)(\psi-\psi_0)\big]\Big\|\\
&\le \Big\|\phi_0^2 f(\psi) - \phi_0^2 f(\psi_0) - \phi_0^2 D_\psi f(\psi_0)(\psi-\psi_0)\Big\|_{H^1(\mathbb{R})}\\
&+ \Big\|\phi^2 f(\psi) - \phi_0^2 f(\psi) - 2\phi_0(\phi-\phi_0) f(\psi)\Big\|_{H^1(\mathbb{R})}\\
&+ \Big\|2\phi_0(\phi-\phi_0)(f(\psi)-f(\psi_0))\Big\|_{H^1(\mathbb{R})}.
\end{aligned}$$

So, using the fact that $\|fg\|_{H^1(\mathbb{R})} \le C\|f\|_{H^1(\mathbb{R})}\,\|g\|_{H^1(\mathbb{R})}$ for some constant C, we find

$$\begin{aligned}
&\Big\|\phi^2 f(\psi) - \phi_0^2 f(\psi_0) - D_{\phi,\psi}\big(\phi^2 f(\psi)\big)\Big|_{(\phi,\psi)=(\phi_0,\psi_0)}\big((\phi-\phi_0),(\psi-\psi_0)\big)\Big\|_{H^1(\mathbb{R})}\\
&\le C\|\phi_0^2\|_{H^1(\mathbb{R})}\Big\|f(\psi) - f(\psi_0) - D_\psi f(\psi_0)(\psi-\psi_0)\Big\|_{H^1(\mathbb{R})}\\
&+ C\|f(\psi)\|_{H^1(\mathbb{R})}\Big\|\phi^2 - \phi_0^2 - 2\phi_0(\phi-\phi_0)\Big\|_{H^1(\mathbb{R})}\\
&+ C\|2\phi_0\|_{H^1(\mathbb{R})}\|\phi-\phi_0\|_{H^1(\mathbb{R})}\|f(\psi)-f(\psi_0)\|_{H^1(\mathbb{R})}.
\end{aligned}$$

The result now follows quickly, since

$$\Big\|(\phi-\phi_0,\psi-\psi_0)\Big\|_{H^1(\mathbb{R})\times H^1(\mathbb{R})} = \sqrt{\|\phi-\phi_0\|^2_{H^1(\mathbb{R})} + \|\psi-\psi_0\|^2_{H^1(\mathbb{R})}},$$

is larger than both $\|\phi-\phi_0\|_{H^1(\mathbb{R})}$ and $\|\psi-\psi_0\|_{H^1(\mathbb{R})}$ individually. □

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