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Multiscale analysis of discrete nonlinear evolution equations

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Abstract. The method of multiscale analysis is constructed for discrete systems of evolution equations for which the problem is that of the far behaviour of an input boundary datum. Discrete *slow space variables* are introduced in a general setting and the related finite differences are constructed. The method is applied to a series of representative examples: the Toda lattice, the nonlinear Klein–Gordon chain, the Takeno system and a discrete version of the Benjamin–Bona–Mahoney–Peregrini equation. Among the resulting limit models we find a discrete nonlinear Schrödinger equation (with reversed spacetime), a three-wave resonant interaction system and a discrete modified Volterra model.

1. Introduction

The study of nonlinear dispersive waves, historically originating in water wave problems, has received considerable attention as a consequence of two fundamental discoveries. The first is the concept of complete integrability of partial differential equations discovered for the Korteweg–de Vries equation [1] and soon extended to the nonlinear Schrödinger [2] and sine–Gordon [3] equations (for a review see [4–6]). The second is the modulational instability of wave trains [7] which is a mechanism for the creation of localized nonlinear solitary waves, the solitons [8].

These two discoveries have a common origin, the reductive perturbation method (or multiscale analysis) [9] allowing the deduction of simplified equations from a basic model without losing its characteristic features. The method consists essentially in an asymptotic analysis of a perturbation series, based on the existence of different scales. More specifically, the method generates a hierarchy of (small) scales for the space and time variations of the envelopes of a fundamental (linear) plane wave and all the overtones. The scale is, moreover, directly related to the (small) amplitude of the wave itself. The scaling of variables is performed via a Taylor expansion the frequency $\omega(k)$ in powers of a small deviation of the wavenumber $k = k_0 + \epsilon\kappa$. This deviation from the linear dispersion relation is, of course, generated by the nonlinearity.

The success of the method relies mainly on the nice property that the resulting reduced models are simple, representative and often integrable. *Simple* here means actually simpler than the master equations and allowing for useful information. *Representative* means that they illustrate effectively real processes. This property relies on the self-consistency of the perturbation series which treats all overtones and avoids secularities [10, 11]. *Integrable* means that they carry an infinite set of conserved quantities, have a bi-Hamiltonian formulation, are solvable (in some sense), etc. Finally, as emphasized in [12], there exists a general property of

the reductive perturbation approach which allows us to understand, in a qualitative way, why the reduced systems are *often* integrable.

The situation is quite different in the case of nonlinear lattices (continuous time and discrete space) for which a reductive perturbative method does not exist which would produce reduced *discrete* systems. There are actually three different approaches to multiscale analysis for a discrete evolution. The first is obviously to go to the continuous limit right in the starting system, for which discreteness effects are wiped out. The second is the *semi-discrete* approach which consists in having a discrete carrier wave modulated by a continuous envelope [13]. In the latter case some discreteness aspects are preserved, in particular, the resulting modulational instability may depend on the carrier frequency. The third stems from the adiabatic approximation, but the approach requires one to use the *rotating wave approximation* to artificially eliminate the overtones. The price to pay is that the predictions, for example the modulational instability, are not trustworthy for large times [14].

We propose here a set of tools which allow us to perform multiscale analysis on a discrete evolution equation when the problem is that of the propagation of a signal sent at one end of a nonlinear lattice. These tools rely on the definition of a large grid scale via the comparison of the magnitude of the related difference operator, and on the expansion of the wavenumber in powers of frequency variations due to nonlinearity.

The method will be illustrated in a series of examples (Toda lattice, anharmonic Klein–Gordon chain, Benjamin–Bona–Mahoney–Peregrini (BBMP) equation, . . .) for which the reduced model for the slowly varying envelope $\psi(n, t)$ results in the following evolution (over dot stands for partial time derivative)

$$-i\beta[\psi_{n+1} - \psi_{n-1}] + \alpha\ddot{\psi}_n - \gamma|\psi_n|^2\psi_n = 0. \quad (1.1)$$

The coefficients α , β and γ depend on the starting model equation and on the frequency of the carrier wave. The continuous version is well known to apply to pulse propagation in a nonlinear Kerr medium (optical fibre) [15] and has also been obtained in the context of Rayleigh–Taylor instability and electron-beam plasma [16] and referred to there as the *unstable nonlinear Schrödinger* equation.

Another example deals with the Takeno model of exciton–phonon coupling in diatomic chains [17] for which we investigate the three-wave resonant interaction. The resulting discrete system reads

$$\begin{aligned} \dot{X} + v\frac{1}{2}[X_{m+1} - X_{m-1}] &= -\frac{2}{\Omega}a_1\bar{a}_2 \\ \dot{a}_1 + v_1\frac{1}{2}[a_{1,m+1} - a_{1,m-1}] &= \frac{1}{v_1}a_2X \\ \dot{a}_2 + v_2\frac{1}{2}[a_{2,m+1} - a_{2,m-1}] &= -\frac{1}{v_2}a_1\bar{X} \end{aligned} \quad (1.2)$$

where X is the envelope of the phonon wave (carrier frequency Ω , group velocity v), a_j are the envelopes of the two components of the exciton wave (carrier frequencies v_j , group velocities v_j), for the Brillouin selection rule $v_1 - v_2 = \Omega$.

We also illustrate the method by investigating the low-frequency discrete limit of the Toda lattice [18], and obtain

$$u_{n+1} - u_{n-1} + u_n\dot{u}_n = 0 \quad (1.3)$$

which can be viewed as the Volterra model [19] with space and time exchanged.

In this paper, the emphasis will be put mainly on the method and on the above-mentioned simple examples, but not on the physical implications that one can infer from the reduced systems. Indeed, such studies essentially depend on the physical context and thus require

specific attention. After a short statement of the problem in the next section, section 3 is devoted to the definition of the main tools. Section 4 deals with the slowly varying envelope limit of the Toda lattice and section 5 with the nonlinear Klein–Gordon (or sine–Gordon) chain. Section 6 deals with a new nonlinear evolution constructed as a discrete version of the BBMP equation and section 7 is devoted to the study of the three-wave resonant interaction in the Takeno model.

2. Discrete waves

2.1. Boundary value problem

Our purpose is the study of a nonlinear dispersive chain with dispersion relation $\Omega(K)$. The physical problem we are concerned with is the following: the first particle of the chain (say $n = 0$) is given an oscillation (or is submitted to an external force) at frequency Ω . In a linear chain this oscillation would propagate without distortion as the plane wave $\exp[i\Omega t + Knd]$, where d is the lattice spacing.

However, the nonlinearity induces some deviations from the value Ω , namely, the wave propagates with actual frequency ω and wavenumber k that we define as

$$\omega = \Omega + \epsilon v \quad (2.1)$$

and by Taylor expansion

$$k = K + \epsilon \frac{1}{c} v + \epsilon^2 \gamma v^2 \quad (2.2)$$

for the following definitions (note that c is the group velocity at K)

$$\frac{1}{c} = \left. \frac{\partial k}{\partial \omega} \right|_{\Omega} \quad 2\gamma = \left. \frac{\partial^2 k}{\partial \omega^2} \right|_{\Omega}. \quad (2.3)$$

For notation simplicity, we shall assume here that $\gamma = 1$, which does not reduce the generality of our task.

A wavepacket in the *linear case* is then given by the Fourier transform

$$u_n(t) = \int d\omega \hat{u}(\omega) e^{i(\omega t + knd)}$$

where $\hat{u}(\omega)$ has support inside the allowed band frequency $[\omega_0, \omega_b]$, which gives here

$$u_n(t) = \epsilon e^{i(\Omega t + Knd)} \int dv \hat{u}(v) e^{iv\epsilon(t+nd/c)} e^{iv^2\epsilon^2 nd}$$

or else

$$u_n(t) = A(n, t) \psi(\xi_n, \tau_n) \quad \begin{cases} A(n, t) = e^{i(\Omega t + Knd)} \\ \psi(\xi_n, \tau_n) = \epsilon \int dv \hat{u}(v) e^{i(v\tau_n + v^2\xi_n d)} \end{cases} \quad (2.4)$$

by means of the following change of *independent variables*:

$$\tau_n = \epsilon(t + nd/c) \quad \xi_n = \epsilon^2 n. \quad (2.5)$$

2.2. Discrete scaling

In order to keep discreteness in the space variable for the envelope $\psi(\xi_n, \tau_n)$, we fix the small parameter as

$$\epsilon^2 = 1/N \quad (2.6)$$

and, for any given n , we shall consider only the set of points $\{\dots, n - N, n, n + N, \dots\}$ of a large grid indexed by the slow variable m , that is

$$\dots, (n - N) \rightarrow (m - 1), n \rightarrow m, (n + N) \rightarrow (m + 1), \dots \quad (2.7)$$

To simplify the notation, we shall be using everywhere

$$\psi(\xi_j, \tau_j) = \tilde{\psi}_j \quad \psi(\xi_j, \tau_n) = \psi_j \quad (2.8)$$

for a given n and all j (note that $\tilde{\psi}_n = \psi_n$). Hence we are interested in expressing everything in terms of $\psi_m = \psi(m, \tau)$ defined as

$$\psi_{n-N} = \psi_{m-1} \quad \psi_n = \psi_m \quad \psi_{n+N} = \psi_{m+1}. \quad (2.9)$$

The problem is now to express the various difference operators occurring in nonlinear evolutions for the product $A(n, t)\psi_m$ in terms of difference operators for ψ_m .

2.3. Initial value problem

The traditional approach to multiscaling for continuous media originates from water wave theory for which the physical problem is usually that of the evolution of an initial disturbance (e.g. of the surface). In this case the observer has to follow the deformation at the (linear) group velocity.

This operation corresponds to making, in the general Fourier transform solution, the expansion of $\omega(k)$ around small deviations of k from the linear dispersion law. The resulting change of variables (in the discrete case for comparison) would then read

$$\tau_n = \epsilon^2 t \quad \xi_n = \epsilon(nd + ct) \quad (2.10)$$

which indeed corresponds to a translation at the group velocity c that is in the *co-moving frame*.

In this case, the change of variable definitely breaks the discreteness of the space variable. Hence, an initial value problem for a discrete lattice in continuous time cannot be treated within a fully discrete multiscale analysis.

However, when the phenomenon to observe results from a boundary input datum, the observer stands at some given point of the lattice and compares the received signal with the input signal. This has to be done in the *retarded time*, which corresponds to the change of variables (2.5), and obviously does not destroy the discrete character of the variables.

3. Difference operators

3.1. General consideration

Before going to the technical points, it is quite useful to recall elementary facts concerning the relation between continuous derivation and discrete differences. Let ϕ_n denote a function of the discrete variable n which varies slowly from one site to the other. In that case we can represent this function by the function $f(x) = \phi_n$ of the continuous variable $x = nd$. The constant d is a *small arbitrary* real number which does not need to be related to the dimension of the grid spacing (this would be necessary if $f(x)$ would be the datum and ϕ_n its representation). By Taylor expansion we readily obtain

$$d \frac{\partial f(x)}{\partial x} = \phi_{n+1} - \phi_n + \mathcal{O}(d^2) \quad (3.1)$$

$$d \frac{\partial f(x)}{\partial x} = \frac{1}{2}[\phi_{n+1} - \phi_{n-1}] + \mathcal{O}(d^3) \quad (3.2)$$

$$d^2 \frac{\partial^2 f(x)}{\partial x^2} = \phi_{n+1} - 2\phi_n + \phi_{n-1} + \mathcal{O}(d^4). \quad (3.3)$$

Consequently, if the precision of the first derivative has to exceed at least the value of the second derivative, it has to be defined with (3.2). This is not the only reason for considering centred differences. The first-order wave equation

$$\partial_t \phi_n - v \frac{1}{2} [\phi_{n+1} - \phi_{n-1}] = 0$$

possesses a *good* dispersion relation ($\omega = v \sin k$) with real-valued solution. Such would not be the case with definition (3.1).

Going now to the stretched space variable $\xi = \epsilon^2 x$, we readily get

$$\phi_{n\pm 1} = \phi_n \pm \epsilon^2 d \frac{\partial f(\xi)}{\partial \xi} + \epsilon^4 \frac{1}{2} d^2 \frac{\partial^2 f(\xi)}{\partial \xi^2} \pm \epsilon^6 \frac{1}{6} d^3 \frac{\partial^3 f(\xi)}{\partial \xi^3} + \dots$$

which, under the discretization procedure according to the rules (3.2) and (3.3), leads to the following *qualitative indications* for the change of variable on the first and second derivatives

$$\phi_{n+1} - \phi_{n-1} = \epsilon^2 [\phi_{m+1} - \phi_{m-1}] + \mathcal{O}(\epsilon^6) \tag{3.4}$$

$$\phi_{n+1} - 2\phi_n + \phi_{n-1} = \epsilon^4 [\phi_{m+1} - 2\phi_m + \phi_{m-1}] + \mathcal{O}(\epsilon^8). \tag{3.5}$$

3.2. Construction of the stretched grid

For $\epsilon^2 = 1/N$, the above expressions serve as a guide to the correct rules for the change of coordinates. They can be understood simply within the definitions (2.6) and (2.7) by writing

$$\begin{aligned} \phi_{n+N} - \phi_{n-N} &= (\phi_{n+N} - \phi_{n+N-2}) + (\phi_{n+N-2} - \phi_{n+N-4}) \\ &+ \dots + (\phi_{n-N+4} - \phi_{n-N+2}) + (\phi_{n-N+2} - \phi_{n-N}) \sim N[\phi_{n+1} - \phi_{n-1}] \end{aligned}$$

where N has to be chosen odd so as to find in the above expansion the very term $\phi_{n+1} - \phi_{n-1}$. Then the meaning of this grid change is that, on the interval $[n - N, n + N]$, the variations of ϕ_n are almost equal, or else that ϕ_n is of almost constant slope (with a precision of $1/N^2$). The purpose now is to construct rigorously such simple rules, and in particular to determine the conditions of *slow variation* under which expressions like (3.4) and (3.5) do hold.

To that end, we define the derivatives in the original variable n as (the C_k^ℓ are the binomial coefficients $k!/\ell!(k - \ell)!$)

$$\nabla \phi_n = \phi_{n+1} - \phi_{n-1} \quad \nabla^k \phi_n = \sum_{\ell=0}^k (-)^\ell C_k^\ell \phi_{n+k-2\ell} \tag{3.6}$$

and the derivatives in the new variable m defined in (2.7) as

$$\Delta_N \phi_n = \phi_{n+N} - \phi_{n-N} \quad \Delta_N^k \phi_n = \sum_{\ell=0}^k (-)^\ell C_k^\ell \phi_{n+N(k-2\ell)}. \tag{3.7}$$

By expressing the value of a function ϕ_n at any other point $n + N$ in terms of the differences $\nabla^k \phi_n$ up to $k = N$, we prove [20] in the appendix that for any odd $N = 2q + 1$

$$\Delta_N \phi_n = \sum_{\ell=0}^q \alpha_q^\ell \nabla^{2\ell+1} \phi_n \quad \alpha_q^\ell = \frac{(2q + 1)(q + \ell)!}{(q - \ell)!(2\ell + 1)!} \tag{3.8}$$

$$\Delta_N^2 \phi_n = \sum_{\ell=1}^{2q+1} \gamma_q^\ell \nabla^{2\ell} \phi_n \quad \gamma_q^\ell = \frac{2(2q + 1)(2q + \ell)!}{(2q + 1 - \ell)!(2\ell)!}. \tag{3.9}$$

The above expressions are *identities* which replace the analogue continuous change of variable $\partial_x \phi = \epsilon^2 \partial_\xi \phi$. Note that the first coefficients are $\alpha_q^0 = N$ and $\gamma_q^1 = N^2$. In general the p th order Δ_N difference will have the first term $N^p \nabla^p \phi_n$.

3.3. *Slow variables*

We now make the hypothesis of *slow variation* of the function ϕ_n as

$$|\nabla^{k+1}\phi_n| = \epsilon^2 |\nabla^k \phi_n| + \mathcal{O}(\epsilon^4) \tag{3.10}$$

for some norm. Such a hypothesis is never explicit in the continuous case where it is usually *admitted implicitly* that, if $\partial_x \phi = \epsilon^2 \partial_\xi \phi$, then $|\partial_x^2 \phi| \sim \epsilon^2 |\partial_x \phi|$. However, in fact it goes the other way round: first one must assume that the function $\phi(x)$ is of slow variation in x , i.e.

$$\left| \frac{\partial^{k+1}\phi}{\partial x} \right| \sim \epsilon^2 \left| \frac{\partial^k \phi}{\partial x} \right|$$

and second it is this very measure ϵ^2 of the *velocity of variation* of $\phi(x)$ that allows us to make the change of variable $\xi = \epsilon^2 x$.

It is necessary now to check that the hypothesis of slow variation is compatible with the expression (3.8) and (3.9) as soon as N is chosen equal (nearest odd integer) to ϵ^{-2} . By a recursive use of (3.10) we obtain the following majorations at large $N = 2q + 1$:

$$\frac{1}{N} |\Delta_N \phi_n| < |\nabla \phi_n| \sum_{\ell=0}^q \frac{\alpha_q^\ell}{(2q+1)^{2\ell+1}}$$

$$\frac{1}{N^2} |\Delta_N^2 \phi_n| < |\nabla^2 \phi_n| \sum_{\ell=1}^{2q+1} \frac{\gamma_q^\ell}{(2q+1)^{2\ell}}$$

We compute the sums of the above series as $N = 2q + 1 \rightarrow \infty$:

$$\lim_{q \rightarrow \infty} \sum_{\ell=0}^q \frac{\alpha_q^\ell}{(2q+1)^{2\ell+1}} = \sum_{\ell=0}^{\infty} \frac{1}{2^{2\ell} (2\ell+1)!} = 2 \sinh\left(\frac{1}{2}\right) = 1.042 \tag{3.11}$$

$$\lim_{q \rightarrow \infty} \sum_{\ell=1}^{2q+1} \frac{\gamma_q^\ell}{(2q+1)^{2\ell}} = \sum_{\ell=1}^{\infty} \frac{2}{(2\ell)!} = 2 \cosh(1) - 2 = 1.086. \tag{3.12}$$

Hence the slow variation assumptions are compatible with the series (3.8) and (3.9). The convergence is actually quite fast as, for example in the order one difference, the first correction coefficient is $1/24$ to be compared to $2 \sinh(1/2) - 1$ (they differ by 0.5×10^{-3}).

Now, with the assumption (3.10), the identities (3.8) and (3.9) together with $1/N = \epsilon^2$, $N = 2q + 1$, lead to

$$\nabla \phi_n = \frac{1}{N} \Delta_N \phi_n + \mathcal{O}(1/N^3) \quad \nabla^2 \phi_n = \frac{1}{N^2} \Delta_N^2 \phi_n + \mathcal{O}(1/N^4) \tag{3.13}$$

which are the general rules for the change of variable $n \rightarrow m$ in the first and second differences. These rules do concur with (3.4) and (3.5).

3.4. *General expressions*

Remembering the notation (2.8), by Taylor expansion in the continuous variable τ_n , we have

$$\tilde{\psi}_{n+1} = \psi_{n+1} + \epsilon \frac{d}{c} \partial_\tau \psi_{n+1} + \frac{1}{2} \left(\epsilon \frac{d}{c}\right)^2 \partial_\tau^2 \psi_{n+1} + \frac{1}{6} \left(\epsilon \frac{d}{c}\right)^3 \partial_\tau^3 \psi_{n+1}$$

$$\tilde{\psi}_{n-1} = \psi_{n-1} - \epsilon \frac{d}{c} \partial_\tau \psi_{n-1} + \frac{1}{2} \left(\epsilon \frac{d}{c}\right)^2 \partial_\tau^2 \psi_{n-1} - \frac{1}{6} \left(\epsilon \frac{d}{c}\right)^3 \partial_\tau^3 \psi_{n-1}.$$

Then we use the identities (such general expressions are given in the appendix)

$$\psi_{n+1} - \psi_n = \frac{1}{2} [\psi_{n+1} - \psi_{n-1}] + \frac{1}{2} [\psi_{n+1} - 2\psi_n + \psi_{n-1}]$$

$$\psi_n - \psi_{n-1} = \frac{1}{2} [\psi_{n+1} - \psi_{n-1}] - \frac{1}{2} [\psi_{n+1} - 2\psi_n + \psi_{n-1}]$$

to replace hereabove ψ_{n+1} and ψ_{n-1} in terms of ψ_n . Finally, by means of (3.13) we arrive at the following general expressions which constitute the basic tool which allows computation of the first and second derivatives:

$$\begin{aligned} \tilde{\psi}_{n+1} = & \psi_m + \epsilon \frac{d}{c} \partial_\tau \psi_m + \frac{1}{2} \epsilon^2 \left(\frac{d}{c}\right)^2 \partial_\tau^2 \psi_m + \frac{1}{N} \frac{1}{2} [\psi_{m+1} - \psi_{m-1}] \\ & + \frac{\epsilon}{N} \frac{d}{c} \frac{1}{2} \partial_\tau [\psi_{m+1} - \psi_{m-1}] + \frac{1}{6} \epsilon^3 \left(\frac{d}{c}\right)^3 \partial_\tau^3 \psi_m + \frac{1}{2N^2} [\psi_{m+1} - 2\psi_m + \psi_{m-1}] \\ & + \frac{\epsilon^2}{4N} \left(\frac{d}{c}\right)^2 \partial_\tau^2 [\psi_{m+1} - \psi_{m-1}] + \frac{\epsilon^4}{24} \left(\frac{d}{c}\right)^4 \partial_\tau^4 \psi_m + \mathcal{O}(\epsilon^5) \end{aligned} \quad (3.14)$$

$$\begin{aligned} \tilde{\psi}_{n-1} = & \psi_m - \epsilon \frac{d}{c} \partial_\tau \psi_m + \frac{1}{2} \epsilon^2 \left(\frac{d}{c}\right)^2 \partial_\tau^2 \psi_m - \frac{1}{N} \frac{1}{2} [\psi_{m+1} - \psi_{m-1}] \\ & + \frac{\epsilon}{N} \frac{d}{c} \frac{1}{2} \partial_\tau [\psi_{m+1} - \psi_{m-1}] - \frac{1}{6} \epsilon^3 \left(\frac{d}{c}\right)^3 \partial_\tau^3 \psi_m + \frac{1}{2N^2} [\psi_{m+1} - 2\psi_m + \psi_{m-1}] \\ & - \frac{\epsilon^2}{4N} \left(\frac{d}{c}\right)^2 \partial_\tau^2 [\psi_{m+1} - \psi_{m-1}] + \frac{\epsilon^4}{24} \left(\frac{d}{c}\right)^4 \partial_\tau^4 \psi_m + \mathcal{O}(\epsilon^5). \end{aligned} \quad (3.15)$$

Note that pushing the general formula (3.13) to higher orders, we can reach any order of precision in such expansions.

3.5. Discrete derivative of a function

By straightforward calculations, using the above basic formulae (3.14) and (3.15), the first derivative follows

$$\tilde{\psi}_{n+1} - \tilde{\psi}_{n-1} = 2\epsilon \frac{d}{c} \partial_\tau \psi_m + \frac{1}{N} [\psi_{m+1} - \psi_{m-1}] + \mathcal{O}(\epsilon^3) \quad (3.16)$$

together with the second derivative

$$\begin{aligned} \tilde{\psi}_{n+1} - 2\tilde{\psi}_n + \tilde{\psi}_{n-1} = & \epsilon^2 \left(\frac{d}{c}\right)^2 \partial_\tau^2 \psi_m + \frac{\epsilon}{N} \frac{d}{c} \partial_\tau [\psi_{m+1} - \psi_{m-1}] \\ & + \frac{1}{N^2} [\psi_{m+1} - 2\psi_m + \psi_{m-1}] + \frac{\epsilon^4}{12} \left(\frac{d}{c}\right)^4 \partial_\tau^4 \psi_m + \mathcal{O}(\epsilon^5). \end{aligned} \quad (3.17)$$

It is worth remarking that, by continuation of the above formulae stopped at ϵ^3 for the first derivative and at order ϵ^4 for the second, we obtain

$$\begin{aligned} \frac{\partial}{\partial x} = & \epsilon^2 \frac{\partial}{\partial \xi} + \frac{\epsilon}{c} \frac{\partial}{\partial \tau} + \theta(\epsilon^3) \\ \frac{\partial^2}{\partial x^2} = & 2 \frac{\epsilon^3}{c} \frac{\partial}{\partial \tau} \frac{\partial}{\partial \xi} + \frac{\epsilon^2}{c^2} \frac{\partial^2}{\partial \tau^2} + \theta(\epsilon^4) \end{aligned}$$

which are the very relations corresponding to the change of variables

$$\tau = \epsilon(t + x/c) \quad \xi = \epsilon^2 x$$

the continuous analogue of (2.5).

3.6. Discrete derivative of a product

We now have to obtain the analogous relations for the product

$$u_n(t) = A(n, t) \psi(\xi_n, \tau_n) = A_n \tilde{\psi}_n$$

appearing in definition (2.4). The quantity $u_{n+1} - u_{n-1}$ is factorized as

$$A_{n+1}\tilde{\psi}_{n+1} - A_{n-1}\tilde{\psi}_{n-1} = \frac{1}{2}[A_{n+1} - A_{n-1}][\tilde{\psi}_{n+1} + \tilde{\psi}_{n-1}] + \frac{1}{2}[A_{n+1} + A_{n-1}][\tilde{\psi}_{n+1} - \tilde{\psi}_{n-1}]$$

and using the basic formula (3.14) and (3.15), it follows at order ϵ/N or ϵ^3

$$\begin{aligned} u_{n+1} - u_{n-1} &= [A_{n+1} - A_{n-1}]\psi_m + \epsilon \frac{d}{c}[A_{n+1} + A_{n-1}]\partial_\tau \psi_m + \frac{1}{N} \frac{1}{2}[A_{n+1} + A_{n-1}] \\ &\quad \times [\psi_{m+1} - \psi_{m-1}] + \epsilon^2 \left(\frac{d}{c}\right)^2 \frac{1}{2}[A_{n+1} - A_{n-1}]\partial_\tau^2 \psi_m. \end{aligned} \quad (3.18)$$

The second derivative is factorized as follows

$$\begin{aligned} u_{n+1} - 2u_n + u_{n-1} &= \frac{1}{2}[A_{n+1} - A_{n-1}][\tilde{\psi}_{n+1} - \tilde{\psi}_{n-1}] \\ &\quad + \frac{1}{2}[A_{n+1} + A_{n-1}][\tilde{\psi}_{n+1} - 2\tilde{\psi}_n + \tilde{\psi}_{n-1}] + \tilde{\psi}_n[A_{n+1} - 2A_n + A_{n-1}] \end{aligned}$$

which readily gives from (3.14) and (3.15)

$$\begin{aligned} u_{n+1} - 2u_n + u_{n-1} &= [A_{n+1} - 2A_n + A_{n-1}]\psi_m + \epsilon[A_{n+1} - A_{n-1}]\frac{d}{c}\partial_\tau \psi_m \\ &\quad + \epsilon^2 \frac{1}{2}[A_{n+1} + A_{n-1}]\left(\frac{d}{c}\right)^2 \partial_\tau^2 \psi_m + \frac{1}{N} \frac{1}{2}[A_{n+1} - A_{n-1}][\psi_{m+1} - \psi_{m-1}] \end{aligned} \quad (3.19)$$

at order ϵ/N or ϵ^3 . The formulae (3.18) and (3.19) constitute our basic tool for deriving reduced models in the following sections.

4. The Toda lattice

The Toda chain is defined by the equation [18]

$$\ddot{x}_n = e^{x_{n+1} - x_n} - e^{x_n - x_{n-1}} \quad (4.1)$$

which can also be written

$$\frac{\partial B(n, t)}{\partial t} = [1 + B(n, t)](V(n, t) - V(n - 1, t)) \quad (4.2)$$

$$\frac{\partial V(n, t)}{\partial t} = B(n + 1, t) - B(n, t) \quad (4.3)$$

for the following definitions

$$1 + B(n, t) = e^{x_n - x_{n-1}} \quad V(n, t) = \dot{x}_n. \quad (4.4)$$

The dispersion relation for the linearized version of the above equation

$$\Omega^2 = 4 \sin^2 \frac{Kd}{2} \quad (4.5)$$

is precisely that of the chain of coupled masses.

Following section 2 we expand $\omega = \Omega + \epsilon\nu$ and consider here the two cases $\Omega = 0$ and $\Omega \neq 0$. The case $\Omega = 0$ can be viewed as the low-frequency limit of the Toda chain, which is actually the standard long wave limit. The case $\Omega \neq 0$ corresponds to the slowly varying envelope approximation of solutions of the Toda lattice.

4.1. Slowly varying envelope approximation

We first seek a solution of equations (4.2) and (4.3) in the form of a Fourier expansion in harmonics of the fundamental $A(n, t) = \exp i(\Omega t + Knd)$ where the Fourier components are developed in a Taylor series in powers of the small parameter ϵ measuring the amplitude of the initial wave

$$B(n, t) = \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \psi_p^{(l)}(\xi_n, \tau_n) A^l(n, t) \tag{4.6}$$

$$V(n, t) = \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \phi_p^{(l)}(\xi_n, \tau_n) A^l(n, t). \tag{4.7}$$

Note that the above series includes all overtones $A^l(n, t) = \exp il(\Omega t + Knd)$ up to order p . These are generated by the nonlinear terms which explains that the corresponding coefficients are of maximum order ϵ^p . Here we have the real-valuedness conditions

$$\psi_p^{(-l)} = (\psi_p^{(l)})^* \quad \phi_p^{(-l)} = (\phi_p^{(l)})^* \tag{4.8}$$

the asterisk denoting complex conjugations. The slow variables τ_n and ξ_n are introduced via

$$\tau_n = \epsilon \left(t + \frac{nd}{c} \right) \quad \xi_n = \epsilon^2 n \tag{4.9}$$

where the velocity c will be determined later as a solvability condition of equations (4.2) and (4.3).

By substitution of (4.6) and (4.7) into (4.2) and (4.3) and using (3.18) (together with $\partial_t = \epsilon \partial_\tau$) at order two in ϵ we obtain

$$\sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \epsilon \frac{\partial}{\partial \tau} \psi_p^{(l)}(m, \tau) + i\Omega l \psi_p^{(l)}(m, \tau) \right\} A^l(n, t) \tag{4.10}$$

$$\begin{aligned} &= \left\{ 1 + \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \psi_p^{(l)}(m, \tau) A^l(n, t) \right\} \\ &\times \left\{ \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left[\phi_p^{(l)}(m, \tau) (A^l(n, t) - A^l(n-1, t)) \right. \right. \\ &+ \epsilon \left(\frac{d}{c} \right) \frac{\partial \phi_p^{(l)}(m, \tau)}{\partial \tau} A^l(n-1, t) - \frac{1}{2} \epsilon^2 \left(\frac{d}{c} \right)^2 \frac{\partial^2 \phi_p^{(l)}(m, \tau)}{\partial \tau^2} A^l(n-1, t) \\ &\left. \left. + \epsilon^2 (\phi_p^{(l)}(m+1, \tau) - \phi_p^{(l)}(m-1, \tau)) \frac{1}{2} A^l(n-1, t) + \dots \right] \right\} \end{aligned} \tag{4.11}$$

$$\sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \epsilon \frac{\partial}{\partial \tau} \phi_p^{(l)}(m, \tau) + i\Omega l \phi_p^{(l)}(m, \tau) \right\} A^l(n, t)$$

$$\begin{aligned} &= \sum_{l=-p}^{l=p} \epsilon^p \left\{ \psi_p^{(l)}(m, \tau) (A^l(n+1, t) - A^l(n, t)) \right. \\ &+ \epsilon \left(\frac{d}{c} \right) \frac{\partial \psi_p^{(l)}(m, \tau)}{\partial \tau} A^l(n+1, t) + \frac{1}{2} \epsilon^2 \left(\frac{d}{c} \right)^2 \frac{\partial^2 \psi_p^{(l)}(m, \tau)}{\partial \tau^2} A^l(n+1, t) \\ &\left. + \epsilon^2 (\psi_p^{(l)}(m+1, \tau) - \psi_p^{(l)}(m-1, \tau)) \frac{1}{2} A^l(n+1, t) + \dots \right\}. \end{aligned} \tag{4.12}$$

We can now proceed to collect and solve different orders of ϵ^p and harmonics l , order (p, l) , in (4.10) and (4.12). Note that it is enough to consider $l > 0$ as negative values follow from the reality condition (4.8). In the leading order $(1, l)$ we have

$$\sum_{l=-1}^{l=1} i\Omega l \psi_1^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-1}^{l=1} \phi_1^{(l)}(m, \tau) (A^l(n, t) - A^l(n-1, t)) = 0 \quad (4.13)$$

$$\sum_{l=-1}^{l=1} i\Omega l \phi_1^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) (A^l(n+1, t) - A^l(n, t)) = 0. \quad (4.14)$$

This is a linear homogeneous system for $\psi_1^{(l)}(m, \tau)$ and $\phi_1^{(l)}(m, \tau)$ polynomials in A . Hence, each coefficient has to vanish separately. For $l = 0$ the system gives trivial equations. For $l = 1$ the determinant of the system for $\psi_1^{(1)}(m, \tau)$ and $\phi_1^{(1)}(m, \tau)$ is zero if $\Omega(K)$ verifies the dispersion relation

$$\Omega(K) = 2 \sin \frac{Kd}{2}. \quad (4.15)$$

Under this condition we seek the general non-trivial solution of equations (4.13) and (4.14)

$$\psi_1^{(1)}(m, \tau) = a\eta(m, \tau) \quad \phi_1^{(1)}(m, \tau) = \eta(m, \tau) \quad (4.16)$$

with a given by

$$a = \exp\left(\frac{-iKd}{2}\right). \quad (4.17)$$

At order $(2, l)$ we have the system

$$\begin{aligned} & \sum_{l=-2}^{l=2} \{i\Omega l \psi_2^{(l)}(m, \tau) - \phi_2^{(l)}(m, \tau)(1 - a^{2l})\} A^l(n, t) \\ & + \sum_{l=-1}^{l=1} \left\{ \frac{\partial \psi_1^{(l)}(m, \tau)}{\partial \tau} - \left(\frac{d}{c}\right) \frac{\partial \phi_1^{(l)}(m, \tau)}{\partial \tau} a^{2l} \right\} A^l(n, t) \\ & - \left\{ \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) \times \sum_{l=-1}^{l=1} \phi_1^{(l)}(m, \tau) (1 - a^{2l}) A^l(n, t) \right\} = 0 \end{aligned} \quad (4.18)$$

$$\begin{aligned} & \sum_{l=-2}^{l=2} \{i\Omega l \phi_2^{(l)}(m, \tau) - \psi_2^{(l)}(m, \tau)(a^{-2l} - 1)\} A^l(n, t) \\ & + \sum_{l=-1}^{l=1} \left\{ \frac{\partial \phi_1^{(l)}(m, \tau)}{\partial \tau} - \left(\frac{d}{c}\right) \frac{\partial \psi_1^{(l)}(m, \tau)}{\partial \tau} a^{-2l} \right\} A^l(n, t) = 0. \end{aligned} \quad (4.19)$$

For $l = 0$ we obtain a homogeneous system with non-zero determinant, consequently only the trivial solution exists, so that

$$\psi_1^{(0)}(m, \tau) = 0 \quad \phi_1^{(0)}(m, \tau) = 0. \quad (4.20)$$

For $l = 1$ we have an inhomogeneous linear system for $\psi_2^{(1)}(m, \tau)$ and $\phi_2^{(1)}(m, \tau)$. The determinant of the associated homogeneous system is zero owing to the dispersion relation (4.15). Therefore, the system will have a solution if the Fredholm solvability condition is satisfied, that is if

$$c = \frac{\partial \Omega(K)}{\partial K} = d \cos \frac{Kd}{2} \quad (4.21)$$

which determines c as the group velocity.

Under this solvability condition we get

$$\psi_2^{(1)}(m, \tau) = a\delta(m, \tau) + \frac{a}{i\Omega} \left(a \frac{d}{c} - 1 \right) \frac{\partial \eta(m, \tau)}{\partial \tau} \tag{4.22}$$

$$\phi_2^{(1)}(m, \tau) = \delta(m, \tau) \tag{4.23}$$

where $\delta(m, \tau)$ is an arbitrary function. Furthermore, for $l = 2$ we obtain $\psi_2^{(2)}(m, \tau)$ and $\phi_2^{(2)}(m, \tau)$

$$\psi_2^{(2)}(m, \tau) = \frac{(a\Omega)^2}{2(\Omega^2 - \sin^2 Kd)} \eta^2(m, \tau) \tag{4.24}$$

$$\phi_2^{(2)}(m, \tau) = \frac{\Omega \sin(Kd)}{2(\Omega^2 - \sin^2 Kd)} \eta^2(m, \tau). \tag{4.25}$$

The next order (3, l) gives the system

$$\begin{aligned} & \sum_{l=-3}^{l=3} \{i\Omega l \psi_3^{(l)}(m, \tau) - \phi_3^{(l)}(m, \tau)(1 - a^{2l})\} A^l(n, t) \\ & + \sum_{l=-2}^{l=2} \left\{ \frac{\partial \psi_2^{(l)}(m, \tau)}{\partial \tau} - \left(\frac{d}{c} \right) \frac{\partial \phi_2^{(l)}(m, \tau)}{\partial \tau} a^{2l} + \left(\frac{1}{2} \right) \left(\frac{d}{c} \right)^2 \frac{\partial^2 \phi_1^{(l)}(m, \tau)}{\partial \tau^2} a^{2l} \right. \\ & \left. - [\phi_1^{(l)}(m + 1, \tau) - \phi_1^{(l)}(m - 1, \tau)] \frac{a^{2l}}{2} \right\} A^l(n, t) \\ & - \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) \times \sum_{l=-2}^{l=2} \phi_2^{(l)}(m, \tau)(1 - a^{2l}) A^l(n, t) \\ & - \sum_{l=-2}^{l=2} \psi_2^{(l)}(m, \tau) A^l(n, t) \times \sum_{l=-1}^{l=1} \phi_1^{(l)}(m, \tau)(1 - a^{2l}) A^l(n, t) \\ & - \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) \times \sum_{l=-1}^{l=1} \left(\frac{d}{c} \right) \frac{\partial \phi_1^{(l)}(m, \tau)}{\partial \tau} a^{2l} A^l(n, t) = 0 \tag{4.26} \end{aligned}$$

$$\begin{aligned} & \sum_{l=-3}^{l=3} \{i\Omega l \phi_3^{(l)}(m, \tau) - \psi_3^{(l)}(m, \tau)(a^{-2l} - 1)\} A^l(n, t) \\ & + \sum_{l=-2}^{l=2} \left\{ \frac{\partial \phi_2^{(l)}(m, \tau)}{\partial \tau} - \left(\frac{d}{c} \right) \frac{\partial \psi_2^{(l)}(m, \tau)}{\partial \tau} a^{-2l} \right\} A^l(n, t) \\ & - \sum_{l=-1}^{l=1} \left(\frac{1}{2} \right) \left(\frac{d}{c} \right)^2 \frac{\partial^2 \psi_1^{(l)}(m, \tau)}{\partial \tau^2} a^{2l} A^l(n, t) \\ & - \sum_{l=-1}^{l=1} [\psi_1^{(l)}(m + 1, \tau) - \psi_1^{(l)}(m - 1, \tau)] \frac{a^{2l}}{2} A^l(n, t) = 0. \tag{4.27} \end{aligned}$$

The order (3, 0) allows us to determine $\psi_2^{(0)}(m, \tau)$ and $\phi_2^{(0)}(m, \tau)$ via an inhomogeneous system of equations. They read

$$\psi_2^{(0)}(m, \tau) = \frac{c^2}{c^2 - d^2} |\eta(m, \tau)|^2 \tag{4.28}$$

$$\phi_2^{(0)}(m, \tau) = \frac{cd}{c^2 - d^2} |\eta(m, \tau)|^2. \tag{4.29}$$

The next order (3, 1) is a tedious one which results in the nonlinear evolution for $\eta(m, \tau)$. It is an inhomogeneous linear system of equations for $\psi_3^{(1)}(m, \tau)$ and $\phi_3^{(1)}(m, \tau)$ of determinant zero. Therefore, we will have a solution if the Fredholm solvability condition is satisfied. This condition gives a nonlinear evolution of $\eta(m, \tau)$ in which the term in $\delta(m, \tau)$ coming from $\psi_2^{(1)}(m, \tau)$ and $\phi_2^{(1)}(m, \tau)$ is self-eliminated. The equation for $\eta(m, \tau) = \eta_m$ finally reads

$$-i\beta[\eta_{m+1} - \eta_{m-1}] + \alpha \frac{\partial^2 \eta_m}{\partial \tau^2} - 2|\eta_m|^2 \eta_m = 0 \quad (4.30)$$

with

$$\alpha = \tan^2 \frac{Kd}{2} \quad \beta = \sin Kd. \quad (4.31)$$

4.2. Low-frequency limit

We are interested now in the propagation of a *low-frequency wave* and we define the following quantities

$$\omega = \epsilon v \quad \left. \frac{\partial \omega}{\partial k} \right|_{k=0} = v_g \equiv d \quad (4.32)$$

and then we develop the function $k(\omega)$ in a Taylor series in ϵ . We obtain

$$k = \frac{1}{d}\epsilon v + \gamma \epsilon^3 v^3 \quad \gamma = \left. \frac{1}{6} \frac{\partial^3 k}{\partial \omega^3} \right|_{k=0}. \quad (4.33)$$

From the above expansion, the new variables follow,

$$\tau_n = \epsilon(t + n) \quad \xi_n = \epsilon^3 n \quad (4.34)$$

and consequently we shall consider the *new grid* with the definition

$$\epsilon^3 = \frac{1}{N} \quad \xi_n \rightarrow m \quad \xi_{n+N} \rightarrow m + 1. \quad (4.35)$$

The method and formulae developed before apply identically except that now we have $1/N = \epsilon^3$ instead of ϵ^2 . In particular, the only formula we need to use is that of the second derivative (3.17).

Now we set

$$B_n(t) = \epsilon^2 b(\xi_n, \tau_n) \quad (4.36)$$

and compute the limit expression of the Toda equation (4.4). We obtain

$$\epsilon^4 \partial_\tau \left(\frac{\partial_\tau b(m)}{1 + \epsilon^2 b(m)} \right) = \epsilon^4 \partial_{\tau\tau} b(m) + \epsilon^6 \partial_\tau [b(m+1) - b(m-1)] + \mathcal{O}(\epsilon^8)$$

which finally reduces to

$$b(m+1) - b(m-1) + b(m) \partial_\tau b(m) = 0. \quad (4.37)$$

This equation is a Volterra-like equation where one would have exchanged space and time, as expected.

5. Nonlinear Klein–Gordon chains

The modulation of the solutions of the Toda chain has been shown to obey the nonlinear Schrödinger (NLS)-like equation (1.1) with particular values of the coefficients. It is of interest to compare this situation resulting from an *integrable model* to the one resulting from a *non-integrable* starting equation. Such is the case for the nonlinear Klein–Gordon chain

$$\ddot{u}_n - \omega_1^2(u_{n+1} - 2u_n + u_{n-1}) + \omega_0^2 u_n + \Gamma u_n^3 = 0 \tag{5.1}$$

or the sine–Gordon chain

$$\ddot{u}_n - \omega_1^2(u_{n+1} - 2u_n + u_{n-1}) + \omega_0^2 \sin u_n = 0. \tag{5.2}$$

Both cases, in the perturbation scheme, are equivalent for $\Gamma = -\omega_0^2/6$, and their dispersion relation is

$$\Omega^2 = \omega_0^2 + 4\omega_1^2 \sin^2\left(\frac{Kd}{2}\right). \tag{5.3}$$

5.1. Evolution of the envelope

We start with the evolution (5.1), and seek the evolution of $\psi_m = \psi_1^1$ with the tools developed in section 3 when

$$u(n, t) = \sum_{p=1}^{\infty} \epsilon^p \sum_{\ell=-p}^{\ell=p} e^{i\ell\theta(n,t)} \psi_p^\ell(m, \tau) \tag{5.4}$$

with conditions on ψ_p^ℓ which ensure reality of u_n :

$$\psi_p^\ell = \bar{\psi}_p^{(-\ell)} \quad \psi_p^{(0)} \in \mathbb{R}. \tag{5.5}$$

Here $\theta(n, t) = \Omega t + Knd$, the slow variables are those defined in section 3 (or those used for the Toda chain, namely (4.9)), and we stop everything at order $\epsilon^3 = \epsilon/N$.

The coefficients of the constant term give at order ϵ

$$\omega_0^2 \psi_1^0 \Rightarrow \psi_1^0 = 0$$

at order ϵ^2

$$\omega_0^2 \psi_2^0 \Rightarrow \psi_2^0 = 0$$

and at order ϵ^3

$$(\psi_1^0)_{\tau\tau} - \omega_1^2 \left(\frac{d}{c}\right)^2 (\psi_1^0)_{\tau\tau} + \Gamma[(\psi_1^0)^3 + 6|\psi_1^1|^2 \psi_1^0] + \omega_0^2 \psi_3^0 \Rightarrow \psi_3^0 = 0.$$

The coefficients of $e^{i\theta}$ at order ϵ give

$$\psi_1^1[-\Omega^2 - \omega_1^2(e^{iKd} - 2 + e^{-iKd}) + \omega_0^2] = 0$$

which agrees with the dispersion relation (5.3). Then at order ϵ^2 we obtain

$$\psi_2^1[-\Omega^2 - \omega_1^2(e^{iKd} - 2 + e^{-iKd}) + \omega_0^2] + (\psi_1^1)_\tau \left[2i\Omega - \omega_1^2 \frac{d}{c}(e^{iKd} - e^{-iKd})\right] = 0.$$

The first term in square brackets hereabove vanishes due to the dispersion relation while the second one vanishes too thanks to

$$\Omega = \omega_1^2 \frac{d}{c} \sin Kd \tag{5.6}$$

which is indeed verified as, by definition (2.3),

$$c = \frac{\partial \Omega}{\partial K} = \frac{1}{\Omega} \omega_1^2 d \sin Kd. \quad (5.7)$$

Finally, the order ϵ^3 leads to

$$\begin{aligned} \psi_3^1 [-\Omega^2 - \omega_1^2 (e^{iKd} - 2 + e^{-iKd}) + \omega_0^2] + (\psi_2^1)_\tau \left[2i\Omega - \omega_1^2 \frac{d}{c} (e^{iKd} - e^{-iKd}) \right] \\ + (\psi_1^1)_{\tau\tau} \left[1 - \omega_1^2 \frac{1}{2} \left(\frac{d}{c} \right)^2 (e^{iKd} + e^{-iKd}) \right] \\ - \omega_1^2 \frac{1}{2} (e^{iKd} - e^{-iKd}) [\psi_1^1(m+1) - \psi_1^1(m-1)] + 3\Gamma |\psi_1^1|^2 \psi_1^1. \end{aligned}$$

The first two terms in square brackets hereabove vanish identically and we are left with the equation for $\psi = \psi_1^1$,

$$-i\beta[\psi_{m+1} - \psi_{m-1}] + \alpha \psi_{\tau\tau}(m) + 3\Gamma |\psi_m|^2 \psi_m = 0 \quad (5.8)$$

with the definitions

$$\beta = \omega_1^2 \sin Kd \quad \alpha = 1 - \omega_1^2 \left(\frac{d}{c} \right)^2 \cos Kd. \quad (5.9)$$

The main difference between the parameter values hereabove and those for the (integrable) Toda chain (4.31) is that here α changes sign for some value of K , which is of fundamental importance for the stability properties of the modulation. However, this problem goes beyond the scope of this paper and will be considered elsewhere.

5.2. Continuous limit

In order to check the consistency of our method, it is instructive to examine the continuous limit of the nonlinear Klein–Gordon chain to verify that its (continuous) multiscale analysis gives rise to an equation which is precisely the continuous version of (5.8).

Defining the continuous variable $x = nd$ and the velocity $v = \omega_1 d$, the continuous limit of (5.1) reads

$$u_{tt} - v^2 u_{xx} + \omega_0^2 u + \Gamma u^3 = 0. \quad (5.10)$$

By seeking a solution as a Fourier integral and expanding k in powers of ϵ for $\omega = \Omega + \epsilon v$ around K , we are led as previously to the expansion

$$u(x, t) = \sum_{p=1}^{\infty} \epsilon^p \sum_{\ell=-p}^{\ell=p} e^{i\ell\theta(x,t)} \psi_p^\ell(\xi, \tau) \quad \theta = \Omega t + Kx \quad (5.11)$$

and the change of variables (c is the group velocity at frequency Ω)

$$\xi = \epsilon^2 x \quad \tau = \epsilon \left(t + \frac{x}{c} \right) \quad (5.12)$$

with the reality conditions $\psi_p^\ell = \bar{\psi}_p^{(-\ell)}$.

Inserting everything in the evolution equation (5.10), we obtain as the coefficients of $e^{i\theta}$

$$\begin{aligned} 0 = \epsilon [-\Omega^2 + v^2 K^2 + \omega_0^2] + \epsilon^2 \left[2i\Omega \psi_\tau - 2iK \frac{v^2}{c} \psi_\tau \right] \\ + \epsilon^3 \left[\psi_{\tau\tau} - 2iK v^2 \psi_\xi - \frac{v^2}{c^2} \psi_{\tau\tau} + 3\Gamma A |\psi|^2 \psi \right] + \mathcal{O}(\epsilon^4). \end{aligned}$$

The order ϵ cancels as soon as we select the *linear dispersion relation*

$$\Omega^2 = \omega_0^2 + v^2 K^2. \quad (5.13)$$

The order ϵ^2 then *identically vanishes* as indeed, from the definition of the group velocity, we readily get

$$c = v^2 \frac{K}{\Omega} \Rightarrow i\Omega - \frac{v^2}{c} iK = 0. \quad (5.14)$$

Finally, the order ϵ^3 furnishes

$$-2iKv^2\psi_\xi + \left[1 - \frac{v^2}{c^2}\right]\psi_{\tau\tau} + 3\Gamma|\psi|^2\psi = 0. \quad (5.15)$$

One interesting consequence here is that the coefficient of the second derivative hereabove is from (5.14)

$$1 - \frac{v^2}{c^2} = 1 - \frac{1}{v^2} \frac{\Omega^2}{K^2} = -\frac{\omega_0^2}{v^2 K^2} < 0 \quad (5.16)$$

which never changes sign, in contrast to the discrete case.

With continuous equation (5.10) being the continuous limit of the discrete Klein–Gordon equation (5.1), the consistency check consists now in the verification that the continuous limit of our equation (5.8) is precisely the above NLS equation (5.15). This readily follows from the limits as $Kd \rightarrow 0$:

$$\begin{aligned} \frac{1}{2}[\psi_{m+1} - \psi_{m-1}] &\rightarrow d\psi_\xi \\ \omega_1 d &\rightarrow v \\ \beta = \omega_1^2 \sin Kd &\rightarrow v^2 \frac{K}{d} \\ \alpha = 1 - \frac{(\omega_1 d)^2}{c^2} \cos Kd &\rightarrow 1 - \frac{v^2}{c^2}. \end{aligned}$$

6. Discrete Benjamin–Bona–Mahoney–Peregrini equation

6.1. Construction of the model

From the quite well known Boussinesq equations [21], further asymptotic limits and restriction to unidirectional propagation are possible, leading to reduced models among which we find the Korteweg–de Vries (KdV) equation and the following BBMP equation for the field $u(x, t)$:

$$u_t + u_x - u_{xxt} + uu_x = 0. \quad (6.1)$$

The discrete multiscale tool, unlike in the continuous case, furnishes expressions for the differences as infinite power series in the small parameter. It is always more convenient to stick with the first few orders in the expansion, as in the basic expression (3.16). Consequently, we need to get rid of the third-order derivative in the above evolution by writing instead (6.1) as a system of equations for $u(x, t)$ and two auxiliary fields $p(x, t)$ and $v(x, t)$

$$u_x = p \quad p_t = v \quad v_x - u_t = p(1 + u). \quad (6.2)$$

The discretization of a continuous model is always non-unique. For instance, the discrete analogues of the KdV equation are the Toda lattice or the Langmuir equation, both leading

to the KdV equation in the continuum limit. Among different possible choices, we introduce here the following discrete analogue of (6.2):

$$\begin{aligned} \frac{1}{2}[u(n+1, t) - u(n-1, t)] &= p(n, t) \\ \frac{\partial p(n, t)}{\partial t} &= v(n, t) \\ \frac{1}{2}[v(n+1, t) - v(n-1, t)] - \frac{\partial u(n, t)}{\partial t} &= p(n, t)[1 + u(n, t)]. \end{aligned} \quad (6.3)$$

6.2. Multiscale analysis

As in the Toda case we seek a solution of equations (6.3) in the form of a Fourier expansion in harmonics of the fundamental $A(n, t) = \exp i(\Omega(K)t + Knd)$ and where the Fourier components are developed in a Taylor series in powers of the small parameter ϵ :

$$u(n, t) = \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \eta_p^{(l)}(\xi_n, \tau_n) A^l(n, t) \quad (6.4)$$

$$p(n, t) = \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \psi_p^{(l)}(\xi_n, \tau_n) A^l(n, t) \quad (6.5)$$

$$v(n, t) = \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \phi_p^{(l)}(\xi_n, \tau_n) A^l(n, t). \quad (6.6)$$

The slow variables τ_n and ξ_n are introduced via

$$\tau_n = \epsilon \left(t + \frac{nd}{c} \right) \quad \xi_n = \epsilon^2 n \quad (6.7)$$

where the velocity c will be determined later as a solvability condition.

Using the identities

$$A^l(n+1, t) + A^l(n-1, t) = 2 \cos(Kld) A^l(n, t) \quad (6.8)$$

$$A^l(n+1, t) - A^l(n-1, t) = 2 \sin(Kld) A^l(n, t) \quad (6.9)$$

the discrete derivatives in (6.3) can be written, with the help of the derivative of a product (3.18), as

$$\begin{aligned} \frac{1}{2}(u(n+1, t) - u(n-1, t)) &= \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \eta_p^{(l)}(m, \tau) i \sin(Kld) + \epsilon \left(\frac{d}{c} \right) \frac{\partial \eta_p^{(l)}}{\partial \tau} \cos(Kld) \right. \\ &\quad + \frac{\epsilon^2}{2} [\eta_p^{(l)}(m+1, \tau) - \eta_p^{(l)}(m-1, \tau)] \cos(Kld) \\ &\quad \left. + \frac{\epsilon^2}{2} \left(\frac{d}{c} \right)^2 \frac{\partial^2 \eta_p^{(l)}}{\partial \tau^2} i \sin(Kld) \right\} A^l(n, t) \end{aligned} \quad (6.10)$$

$$\begin{aligned} \frac{1}{2}(v(n+1, t) - v(n-1, t)) &= \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \phi_p^{(l)}(m, \tau) i \sin(Kld) + \epsilon \left(\frac{d}{c} \right) \frac{\partial \phi_p^{(l)}}{\partial \tau} \cos(Kld) \right. \\ &\quad + \frac{\epsilon^2}{2} [\phi_p^{(l)}(m+1, \tau) - \phi_p^{(l)}(m-1, \tau)] \cos(Kld) \\ &\quad \left. + \frac{\epsilon^2}{2} \left(\frac{d}{c} \right)^2 \frac{\partial^2 \phi_p^{(l)}}{\partial \tau^2} i \sin(Kld) \right\} A^l(n, t). \end{aligned} \quad (6.11)$$

Substituting (6.10) and (6.11) in (6.3), we obtain

$$\begin{aligned} \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \eta_p^{(l)}(m, \tau) i \sin(Kld) + \epsilon \left(\frac{d}{c} \right) \frac{\partial \eta_p^{(l)}}{\partial \tau} \cos(Kld) \right. \\ \left. + \frac{\epsilon^2}{2} [\eta_p^{(l)}(m+1, \tau) - \eta_p^{(l)}(m-1, \tau)] \cos(Kld) \right. \\ \left. + \frac{\epsilon^2}{2} \left(\frac{d}{c} \right)^2 \frac{\partial^2 \eta_p^{(l)}}{\partial \tau^2} i \sin(Kld) \right\} A^l(n, t) \\ - \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \psi_p^{(l)}(m, \tau) A^l(n, t) = 0 \end{aligned} \tag{6.12}$$

$$\sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \epsilon \frac{\partial \psi_p^{(l)}(m, \tau)}{\partial \tau} + i\Omega l \psi_p^{(l)}(m, \tau) \right\} A^l(n, t) - \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \phi_p^{(l)}(m, \tau) A^l(n, t) = 0 \tag{6.13}$$

$$\begin{aligned} \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \phi_p^{(l)}(m, \tau) i \sin(Kld) + \epsilon \left(\frac{d}{c} \right) \frac{\partial \phi_p^{(l)}}{\partial \tau} \cos(Kld) \right. \\ \left. + \frac{\epsilon^2}{2} [\phi_p^{(l)}(m+1, \tau) - \phi_p^{(l)}(m-1, \tau)] \cos(Kld) \right. \\ \left. + \frac{\epsilon^2}{2} \left(\frac{d}{c} \right)^2 \frac{\partial^2 \phi_p^{(l)}}{\partial \tau^2} i \sin(Kld) \right\} A^l(n, t) \\ - \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \left\{ \epsilon \frac{\partial \eta_p^{(l)}(m, \tau)}{\partial \tau} + i\Omega l \eta_p^{(l)}(m, \tau) \right\} A^l(n, t) \\ - \left[1 + \sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \eta_p^{(l)}(m, \tau) A^l(n, t) \right] \left[\sum_{l=-p}^{l=p} \sum_{p=1}^{p=\infty} \epsilon^p \psi_p^{(l)}(m, \tau) A^l(n, t) \right] = 0. \end{aligned} \tag{6.14}$$

We proceed now to collect and solve different orders of ϵ^p and harmonics l (order (p, l)) in (6.12)–(6.14). In the leading order $(1, l)$ we have

$$\sum_{l=-1}^{l=1} \eta_1^{(l)}(m, \tau) i \sin(Kld) A^l(n, t) - \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) = 0 \tag{6.15}$$

$$\sum_{l=-1}^{l=1} i\Omega l \psi_1^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-1}^{l=1} \phi_1^{(l)}(m, \tau) A^l(n, t) = 0 \tag{6.16}$$

$$\begin{aligned} \sum_{l=-1}^{l=1} \phi_1^{(l)}(m, \tau) i \sin(Kld) A^l(n, t) - \sum_{l=-1}^{l=1} i\Omega l \eta_1^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) \\ = 0. \end{aligned} \tag{6.17}$$

Equations (6.15), (6.16) and (6.17) constitute a linear homogeneous system for $\eta_1^{(l)}$, $\psi_1^{(l)}$ and $\phi_1^{(l)}$. For $l = 0$, equations (6.15) and (6.16) give

$$\psi_1^{(0)}(m, \tau) = 0 \tag{6.18}$$

$$\phi_1^{(0)}(m, \tau) = 0 \tag{6.19}$$

and (6.17) is satisfied. For $l = 1$ the determinant of the system for $\eta_1^{(1)}$, $\psi_1^{(1)}$ and $\phi_1^{(1)}$ is zero if $\Omega(K)$ verifies the dispersion relation

$$\Omega(K) = -\frac{\sin Kd}{1 + \sin^2 Kd}. \quad (6.20)$$

Under this condition we arrive at the following non-trivial solution of equations (6.15)–(6.17):

$$\eta_1^{(1)}(m, \tau) = \eta(m, \tau) \quad (6.21)$$

$$\psi_1^{(1)}(m, \tau) = i \sin(Kd)\eta(m, \tau) \quad (6.22)$$

$$\phi_1^{(1)}(m, \tau) = \frac{\sin^2 Kd}{1 + \sin^2 Kd} \eta(m, \tau) \quad (6.23)$$

where η is now the unknown function.

At order $(2, l)$ we have the system

$$\begin{aligned} \sum_{l=-2}^{l=2} \eta_2^{(l)}(m, \tau) i \sin(Kld) A^l(n, t) + \sum_{l=-1}^{l=1} \left(\frac{d}{c}\right) \frac{\partial \eta_1^{(l)}(m, \tau)}{\partial \tau} \cos(Kld) A^l(n, t) \\ - \sum_{l=-2}^{l=2} \psi_2^{(l)}(m, \tau) A^l(n, t) = 0 \end{aligned} \quad (6.24)$$

$$\sum_{l=-1}^{l=1} \frac{\partial \psi_1^{(l)}(m, \tau)}{\partial \tau} A^l(n, t) + \sum_{l=-2}^{l=2} i \Omega l \psi_2^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-2}^{l=2} \phi_2^{(l)}(m, \tau) A^l(n, t) = 0 \quad (6.25)$$

$$\begin{aligned} \sum_{l=-2}^{l=2} \phi_2^{(l)}(m, \tau) i \sin(Kld) A^l(n, t) + \sum_{l=-1}^{l=1} \left(\frac{d}{c}\right) \frac{\partial \phi_1^{(l)}}{\partial \tau} \cos(Kld) A^l(n, t) \\ - \sum_{l=-1}^{l=1} \frac{\partial \eta_1^{(l)}(m, \tau)}{\partial \tau} A^l(n, t) - \sum_{l=-2}^{l=2} i \Omega l \eta_2^{(l)}(m, \tau) A^l(n, t) \\ - \sum_{l=-2}^{l=2} \psi_2^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-1}^{l=1} \eta_1^{(l)}(m, \tau) A^l(n, t) \\ \times \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) = 0. \end{aligned} \quad (6.26)$$

For $l = 0$, equation (6.25) gives using (6.18)

$$\phi_2^{(0)}(m, \tau) = 0. \quad (6.27)$$

Under (6.21) and (6.22), equations (6.24) and (6.26) constitute a homogeneous system for $\psi_0^{(2)}$ and the τ derivative of $\eta_1^{(0)}$. The determinant is non-zero and consequently only the trivial solution exists, so that

$$\psi_2^{(0)}(m, \tau) = 0 \quad (6.28)$$

$$\eta_1^{(0)}(m, \tau) = 0. \quad (6.29)$$

For $l = 1$ we have, using (6.25), an inhomogeneous linear system for $\eta_2^{(1)}$ and $\psi_2^{(1)}$. The determinant of the associated homogeneous system is zero owing to the dispersion relation (6.20). Therefore, the system will have a solution for the Fredholm solvability condition, which is satisfied for

$$c = -d \frac{\cos^3(Kd)}{(1 + \sin^2(Kd))^2} = \frac{\partial \Omega}{\partial K} \quad (6.30)$$

which determines c as the group velocity.

It is important to remark here that, for the Taylor expansion (2.2), we must assume a non-vanishing group velocity c as indeed the first term in the expansion of $k(\omega)$ is ϵ/c . Hence, we must avoid here the vicinity of the value $Kd = \pm\pi/2$ for which c vanishes. In that vicinity, one should reconsider the problem completely.

Then for all non-vanishing values of c we get

$$\eta_2^{(1)}(m, \tau) = g(m, \tau) \tag{6.31}$$

$$\psi_2^{(1)}(m, \tau) = ig(m, \tau) \sin(Kd) + \left(\frac{d}{c}\right) \frac{\partial \eta(m, \tau)}{\partial \tau} \cos(Kd) \tag{6.32}$$

$$\phi_2^{(1)}(m, \tau) = -\Omega g(m, \tau) \sin(Kd) + i \frac{\partial \eta(m, \tau)}{\partial \tau} \left(\sin(Kd) - \frac{\tan^2(Kd)}{\Omega} \right) \tag{6.33}$$

where $g(m, \tau)$ is an arbitrary function. Furthermore, for $l = 2$ we obtain $\eta_2^{(2)}$, $\psi_2^{(2)}$ and $\phi_2^{(2)}$ as follows:

$$\eta_2^{(2)}(m, \tau) = a(Kd)\eta^2(m, \tau) \tag{6.34}$$

$$\psi_2^{(2)}(m, \tau) = i \sin(2Kd)a(Kd)\eta^2(m, \tau) \tag{6.35}$$

$$\phi_2^{(2)}(m, \tau) = -2\Omega \sin(2Kd)a(Kd)\eta^2(m, \tau) \tag{6.36}$$

where $a(Kd)$ is defined as

$$a(Kd) = -\frac{\sin(Kd)}{2\Omega[1 + \sin^2(2Kd)] + \sin(2Kd)}. \tag{6.37}$$

The next order (3, l) gives the system

$$\begin{aligned} \sum_{l=-3}^{l=3} \eta_3^{(l)}(m, \tau) i \sin(Kld)A^l(n, t) + \sum_{l=-2}^{l=2} \left(\frac{d}{c}\right) \frac{\partial \eta_2^{(l)}}{\partial \tau} \cos(Kld)A^l(n, t) \\ + \sum_{l=-1}^{l=1} \frac{1}{2} [\eta_1^{(l)}(m+1, \tau) - \eta_1^{(l)}(m-1, \tau)] \cos(Kld)A^l(n, t) \\ + \sum_{l=-1}^{l=1} \frac{1}{2} \left(\frac{d}{c}\right)^2 \frac{\partial^2 \eta_1^{(l)}}{\partial \tau^2} i \sin(Kld)A^l(n, t) - \sum_{l=-3}^{l=3} \psi_3^{(l)}(m, \tau)A^l(n, t) = 0 \end{aligned} \tag{6.38}$$

$$\begin{aligned} \sum_{l=-2}^{l=2} \frac{\partial \psi_2^{(l)}(m, \tau)}{\partial \tau} A^l(n, t) + \sum_{l=-3}^{l=3} i\Omega l \psi_3^{(l)}(m, \tau)A^l(n, t) \\ - \sum_{l=-3}^{l=3} \phi_3^{(l)}(m, \tau)A^l(n, t) = 0 \end{aligned} \tag{6.39}$$

$$\begin{aligned} \sum_{l=-3}^{l=3} \phi_3^{(l)}(m, \tau) i \sin(Kld)A^l(n, t) + \sum_{l=-2}^{l=2} \left(\frac{d}{c}\right) \frac{\partial \phi_2^{(l)}(m, \tau)}{\partial \tau} \cos(Kld)A^l(n, t) \\ + \sum_{l=-1}^{l=1} \frac{1}{2} [\phi_1^{(l)}(m+1, \tau) - \phi_1^{(l)}(m-1, \tau)] \cos(Kld)A^l(n, t) \\ + \sum_{l=-1}^{l=1} \frac{1}{2} \left(\frac{d}{c}\right)^2 \frac{\partial^2 \phi_1^{(l)}(m, \tau)}{\partial \tau^2} i \sin(Kld)A^l(n, t) \\ - \sum_{l=-2}^{l=2} \frac{\partial \eta_2^{(l)}(m, \tau)}{\partial \tau} A^l(n, t) - \sum_{l=-3}^{l=3} i\Omega l \eta_3^{(l)}(m, \tau)A^l(n, t) \end{aligned}$$

$$\begin{aligned}
 & - \sum_{l=-3}^{l=3} \psi_3^{(l)}(m, \tau) A^l(n, t) - \sum_{l=-1}^{l=1} \eta_1^{(l)}(m, \tau) A^l(n, t) \times \sum_{l=-2}^{l=2} \psi_2^{(l)}(m, \tau) A^l(n, t) \\
 & - \sum_{l=-2}^{l=2} \eta_2^{(l)}(m, \tau) A^l(n, t) \times \sum_{l=-1}^{l=1} \psi_1^{(l)}(m, \tau) A^l(n, t) = 0.
 \end{aligned} \tag{6.40}$$

The order (3, 0) determines $\eta_2^{(0)}, \psi_3^{(0)}$ and $\phi_3^{(0)}$ via an inhomogeneous system of equations. They read

$$\eta_2^{(0)}(m, \tau) = -\frac{d \cos(Kd)}{d+c} |\eta(m, \tau)|^2 \tag{6.41}$$

$$\psi_3^{(0)}(m, \tau) = -\left(\frac{d^2}{c}\right) \frac{\cos(Kd)}{d+c} |\eta(m, \tau)|^2 \tag{6.42}$$

$$\phi_3^{(0)}(m, \tau) = 0. \tag{6.43}$$

The next order (3, 1) allows us to find the nonlinear evolution of η . It is an inhomogeneous linear system of equations for $\eta_3^{(1)}, \psi_3^{(1)}$ and $\phi_3^{(1)}$ of determinant zero. Therefore, we will have a solution if the Fredholm solvability condition holds. This condition gives the nonlinear evolution of η in which the term in $g(m, \tau)$ coming from $\eta_2^{(1)}, \psi_2^{(1)}$ and $\phi_2^{(1)}$ cancels out. The equation for $\eta(m, \tau) = \eta_m$ reads finally

$$-i\beta(\eta_{m+1} - \eta_{m-1}) + \alpha \frac{\partial^2 \eta_m}{\partial^2 \tau} - \gamma |\eta_m|^2 \eta_m = 0 \tag{6.44}$$

with the following definitions (we set $Kd = K$ for simplicity)

$$\beta = \frac{1 \cos^3 K \sin K}{2 (1 + \sin^2 K)}$$

$$\alpha = -\frac{1 (\cos^2 K - 1)(\cos^2 K + 6)(\cos^2 K - 2)^2}{2 \cos^4 K}$$

$$\gamma = -\frac{1 \cos^2 K - 28 \cos^6 K + 6 \cos^5 K - 20 \cos^4 K - 11 \cos^3 K + 13 \cos^2 K - 4}{2 \cos^2 K - 4} \frac{4 \cos^3 K + 3 \cos^2 K - \cos K + 1}{4 \cos^3 K + 3 \cos^2 K - \cos K + 1}.$$

Note that in the Brillouin zone $K \in [-\pi, +\pi]$, the coefficient α has a singularity in $K = \pm\pi/2$ where the group velocity vanishes, which is a forbidden region.

7. Three-wave resonant interaction

To further illustrate the method, we consider here the Takeno discrete model for the interaction of excitons (or vibrons) with the phonons in a lattice of coupled harmonic oscillators (via a Frölich-like Hamiltonian) [17]. The model results from the Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{ph}} + \mathcal{H}_{\text{ex}} + \mathcal{H}_{\text{int}} \tag{7.1}$$

$$\mathcal{H}_{\text{ph}} = \frac{1}{2} \sum_n M \dot{u}_n^2 + S [u_{n+1} - u_n]^2$$

$$\mathcal{H}_{\text{ex}} = \frac{1}{2} \sum_n m [\dot{q}_n^2 + \omega_0^2 q_n^2] + s [q_{n+1} - q_n]^2$$

$$\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_n A [u_{n+1} - u_{n-1}] q_n^2. \tag{7.2}$$

After the rescaling

$$q_n = \frac{1}{A} \sqrt{2mM} q'_n \quad u_n = \frac{m}{A} u'_n \tag{7.3}$$

and forgetting the primes, the equations of motion are

$$\begin{aligned} \ddot{u}_n - \Omega_1^2 [u_{n+1} - 2u_n + u_{n-1}] &= q_{n+1}^2 - q_{n-1}^2 \\ \dot{q}_n - \omega_1^2 [q_{n+1} - 2q_n + q_{n-1}] + \omega_0^2 q_n &= -q_n [u_{n+1} - u_{n-1}] \end{aligned} \tag{7.4}$$

with the following definitions:

$$\Omega_1^2 = \frac{S}{M} \quad \omega_1^2 = \frac{s}{m}.$$

7.1. Resonant wave interaction

We consider now the situation of three-wave scattering, that is the situation where the exciton wave contains two components (frequencies ν_1 and ν_2) which interact with the phonon wave (frequency Ω) according to the Brillouin selection rule

$$\nu_1 - \nu_2 = \Omega \quad k_1 - k_2 = K. \tag{7.5}$$

For slowly varying envelopes we set

$$\begin{aligned} q_n(t) = \epsilon [a_1^{(1)} e^{i\theta_1} + a_2^{(1)} e^{i\theta_2}] + \epsilon^2 [a_1^{(2)} e^{2i\theta_1} + a_2^{(2)} e^{2i\theta_2} + a_3^{(2)} e^{2i\phi} + a_4^{(2)} e^{i(\theta_1+\theta_2)} \\ + a_5^{(2)} e^{i(\theta_1+\phi)} + a_6^{(2)} e^{i(\theta_2-\phi)}] + \text{cc} + \mathcal{O}(\epsilon^3) \end{aligned} \tag{7.6}$$

$$\begin{aligned} u_n(t) = \epsilon b_1^{(1)} e^{i\phi} + \epsilon^2 [b_1^{(2)} e^{2i\theta_1} + b_2^{(2)} e^{2i\theta_2} + b_3^{(2)} e^{2i\phi} + b_4^{(2)} e^{i(\theta_1+\theta_2)} + b_5^{(2)} e^{i(\theta_1+\phi)} \\ + b_6^{(2)} e^{i(\theta_2-\phi)}] + \text{cc} + \mathcal{O}(\epsilon^3) \end{aligned} \tag{7.7}$$

where the amplitudes $a_i^{(j)}$ and $b_i^{(j)}$ depend on the slow variables (m, τ) and with the definitions

$$\begin{aligned} \tau = \epsilon t \quad \left\{ \xi_n = \epsilon n \quad \epsilon = \frac{1}{N} \right\} \rightarrow m \\ \theta_1 = k_1 n - \nu_1 t \quad \theta_2 = k_2 n - \nu_2 t \quad \phi = Kn - \Omega t \\ \theta_1 - \theta_2 = \phi. \end{aligned} \tag{7.8}$$

The choice of the above harmonics in the order ϵ^2 results from the remark that quadratic terms (like $q_n u_n$) for three waves induce (with the complex conjugates) waves with phases $2\theta_1, 2\theta_2, 2\phi, \theta_1 + \theta_2, \theta_1 + \phi, \theta_2 + \phi, \theta_1 - \theta_2, \theta_1 - \phi, \theta_2 - \phi$. However, the selection rules give $\theta_2 + \phi = \theta_1, \theta_1 - \theta_2 = \phi, \theta_1 - \phi = \theta_2$, which are already considered at first order and hence need not to be included in the second order.

The above change of variables has to be applied to functions

$$\varphi_n(t) = \psi_m(\tau) e^{i(kn - \omega t)}$$

for which, now using the tools developed in section 3 for $N = \epsilon^{-1}$, we readily obtain at order ϵ

$$\begin{aligned} \ddot{\varphi}_n &= [-\omega^2 \psi_m - \epsilon 2i\omega \partial_\tau \psi_m + \dots] e^{i(kn - \omega t)} \\ \varphi_{n+1} - \varphi_{n-1} &= [2i \sin k \psi_m + \epsilon \cos k (\psi_{m+1} - \psi_{m-1}) + \dots] e^{i(kn - \omega t)} \\ \varphi_{n+1} - 2\varphi_n + \varphi_{n-1} &= [2(\cos k - 1) \psi_m + i\epsilon \sin k (\psi_{m+1} - \psi_{m-1}) + \dots] e^{i(kn - \omega t)}. \end{aligned}$$

7.2. The limit equation

All the above machinery is applied now to the system (7.4) which gives at order ϵ

$$\begin{aligned} e^{i\phi}: \quad & [-\Omega^2 - \Omega_1^2 2(\cos K - 1)] b_1^{(1)} = 0 \\ e^{i\theta_1}: \quad & [-\nu_1^2 - \omega_1^2 2(\cos k_1 - 1) + \omega_0^2] a_1^{(1)} = 0 \\ e^{i\theta_2}: \quad & [-\nu_2^2 - \omega_1^2 2(\cos k_2 - 1) + \omega_0^2] a_2^{(1)} = 0. \end{aligned}$$

These imply the dispersion relations

$$\begin{aligned}\Omega^2 &= 2\Omega_1^2(1 - \cos K) \\ v_1^2 &= \omega_0^2 + 2\omega_1^2(1 - \cos k_1) \quad v_2^2 = \omega_0^2 + \omega_1^2(1 - \cos k_2)\end{aligned}\quad (7.9)$$

and hence the three group velocities

$$v = \frac{\Omega_1^2}{\Omega} \sin K \quad v_1 = \frac{\omega_1^2}{v_1} \sin k_1 \quad v_2 = \frac{\omega_1^2}{v_2} \sin k_2. \quad (7.10)$$

The next order, ϵ^2 , gives in turn

$$\begin{aligned}e^{i\phi}: \quad & -2i\Omega\dot{b}_1^{(1)} - \Omega_1^2 i \sin K [b_{1,m+1}^{(1)} - b_{1,m-1}^{(1)}] = 4i \sin K a_1^{(1)} \bar{a}_2^{(1)} \\ e^{i\theta_1}: \quad & -2iv_1\dot{a}_1^{(1)} - \omega_1^2 i \sin k_1 [a_{1,m+1}^{(1)} - a_{1,m-1}^{(1)}] = -2i \sin K a_2^{(1)} b_1^{(1)} \\ e^{i\theta_2}: \quad & -2iv_2\dot{a}_2^{(1)} - \omega_1^2 i \sin k_2 [a_{2,m+1}^{(1)} - a_{2,m-1}^{(1)}] = 2i \sin K a_1^{(1)} \bar{b}_1^{(1)} \\ e^{2i\theta_1}: \quad & [-4v_1^2 - 2\Omega_1^2(\cos 2k_1 - 1)]b_1^{(2)} = 4i \sin k_1 \cos k_1 [a_1^{(1)}]^2 \\ & : \quad [-4v_1^2 - 2\omega_1^2(\cos 2k_1 - 1) + \omega_0^2]a_1^{(2)} = 0 \\ e^{2i\theta_2}: \quad & [-4v_2^2 - 2\Omega_1^2(\cos 2k_2 - 1)]b_2^{(2)} = 4i \sin k_2 \cos k_2 [a_1^{(2)}]^2 \\ & : \quad [-4v_2^2 - 2\omega_1^2(\cos 2k_2 - 1) + \omega_0^2]a_2^{(2)} = 0 \\ e^{2i\phi}: \quad & [-4\Omega^2 - 2\Omega_1^2(\cos 2K - 1)]b_3^{(2)} = 0 \\ & : \quad [-4\Omega^2 - 2\omega_1^2(\cos 2K - 1) + \omega_0^2]a_3^{(2)} = 0 \\ e^{i(\theta_1+\theta_2)}: \quad & [-4(v_1 + v_2)^2 - 2\Omega_1^2(\cos(k_1 + k_2) - 1)]b_4^{(2)} = 4i \sin(k_1 + k_2)a_1^{(1)}a_2^{(1)} \\ & : \quad [-4(v_1 + v_2)^2 - 2\omega_1^2(\cos(k_1 + k_2) - 1) + \omega_0^2]a_4^{(2)} = 0 \\ e^{i(\theta_1+\phi)}: \quad & [-4(v_1 + \phi)^2 - 2\Omega_1^2(\cos(k_1 + K) - 1)]b_5^{(2)} = 0 \\ & : \quad [-4(v_1 + \phi)^2 - 2\omega_1^2(\cos(k_1 + K) - 1) + \omega_0^2]a_5^{(2)} = -2i \sin K a_1^{(1)} b_1^{(1)} \\ e^{i(\theta_2-\phi)}: \quad & [-4(v_2 - \phi)^2 - 2\Omega_1^2(\cos(k_2 - K) - 1)]b_6^{(2)} = 0 \\ & : \quad [-4(v_2 - \phi)^2 - 2\omega_1^2(\cos(k_2 - K) - 1) + \omega_0^2]a_6^{(2)} = 2i \sin K a_2^{(1)} \bar{b}_1^{(1)}.\end{aligned}$$

The first three equations above provide the evolutions of the envelopes which we scale as

$$X = \sin K b_1^{(1)} \quad a_1 = \sin K a_1^{(1)} \quad a_2 = \sin K a_2^{(1)}$$

and consequently which obey

$$\begin{aligned}\dot{X} + v \frac{1}{2} [X_{m+1} - X_{m-1}] &= -\frac{2}{\Omega} a_1 \bar{a}_2 \\ \dot{a}_1 + v_1 \frac{1}{2} [a_{1,m+1} - a_{1,m-1}] &= \frac{1}{v_1} a_2 X \\ \dot{a}_2 + v_2 \frac{1}{2} [a_{2,m+1} - a_{2,m-1}] &= -\frac{1}{v_2} a_1 \bar{X}.\end{aligned}\quad (7.11)$$

The remaining 12 equations give simply the coefficients of the second harmonics in terms of those of the first, precisely:

$$\begin{aligned}a_1^{(2)} &= a_2^{(2)} = b_3^{(2)} = a_3^{(2)} = a_4^{(2)} = b_5^{(2)} = b_6^{(2)} = 0 \\ b_1^{(2)} &= i \frac{v_1^2 + \frac{1}{2}\Omega_1^2(\cos 2k_1 - 1)}{\sin k_1 \cos k_1} [a_1^{(1)}]^2 \\ b_2^{(2)} &= i \frac{v_2^2 - \frac{1}{2}\Omega_1^2(\cos 2k_2 - 1)}{\sin k_2 \cos k_2} [a_1^{(2)}]^2\end{aligned}$$

$$\begin{aligned}
 b_4^{(2)} &= i \frac{(\nu_1 + \nu_2)^2 + \frac{1}{2}\Omega_1^2(\cos(k_1 + k_2) - 1)}{\sin(k_1 + k_2)} a_1^{(1)} a_2^{(1)} \\
 a_5^{(2)} &= -i \frac{2(\nu_1 + \phi)^2 + \omega_1^2(\cos(k_1 + K) - 1) + \omega_0^2}{\sin K} a_1^{(1)} b_1^{(1)} \\
 a_6^{(2)} &= i \frac{2(\nu_2 - \phi)^2 + \omega_1^2(\cos(k_2 - K) - 1) + \omega_0^2}{\sin K} a_2^{(1)} \bar{b}_1^{(1)}.
 \end{aligned}$$

Hence, equation (7.11) constitute a closed system of equations for the first-order variations of the envelopes. It is the discrete analogue of the continuous three-wave resonant interaction system.

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Appendix. Discrete change of variable

For a given function x of the discrete variable n , we are interested in expressing all-order differences in a *large grid* indexed by the variable m (taking points separated by a given odd integer p) in terms of the original hierarchy of differences (3.6). The following notation will be used throughout:

$$\nabla^\ell x_n = \sum_{k=0}^{\ell} (-)^k C_\ell^k x_{n+\ell-2k} = x_n^{(\ell)} \tag{A.1}$$

$$\Delta_p^\ell x_n = \sum_{k=0}^{\ell} (-)^k C_\ell^k x_{n+p(\ell-2k)} = x_m^{(\ell)}. \tag{A.2}$$

To express the Δ -differences in terms of the ∇ -differences, we first write *exact* Taylor-like series as the following *identities* (valid for any given n and any point function x_n)

$$x_{n+p} = \sum_{j=0}^p a_p^j x_n^{(j)} + \frac{1}{2} \tilde{x}_n^{(p)} \quad x_{n-p} = \sum_{j=0}^p (-)^j a_p^j x_n^{(j)} + (-)^{p+1} \frac{1}{2} \tilde{x}_n^{(p)} \tag{A.3}$$

with the following definitions for the *tilde*-derivatives

$$\tilde{x}_n^{(p)} = x_{n+p} + \sum_{\ell=1}^p (-)^{\ell} C_{p+1}^{\ell} x_{n+p+1-2\ell} + (-)^{p+1} x_{n-p}. \tag{A.4}$$

For instance, we may write

$$\begin{aligned}
 x_{n+5} &= x_n + \frac{5}{2}x_n^{(1)} + \frac{9}{2}x_n^{(2)} + \frac{5}{2}x_n^{(3)} + \frac{6}{2}x_n^{(4)} + \frac{1}{2}x_n^{(5)} + \frac{1}{2}\tilde{x}_n^{(5)} \\
 x_{n+4} &= x_n + \frac{5}{2}x_n^{(1)} + \frac{4}{2}x_n^{(2)} + \frac{5}{2}x_n^{(3)} + \frac{1}{2}x_n^{(4)} + \frac{1}{2}\tilde{x}_n^{(4)} \\
 x_{n+3} &= x_n + \frac{3}{2}x_n^{(1)} + \frac{4}{2}x_n^{(2)} + \frac{1}{2}x_n^{(3)} + \frac{1}{2}\tilde{x}_n^{(3)} \\
 x_{n+2} &= x_n + \frac{3}{2}x_n^{(1)} + \frac{1}{2}x_n^{(2)} + \frac{1}{2}\tilde{x}_n^{(2)} \\
 x_{n+1} &= x_n + \frac{1}{2}x_n^{(1)} + \frac{1}{2}\tilde{x}_n^{(1)} \\
 x_{n-1} &= x_n - \frac{1}{2}x_n^{(1)} + \frac{1}{2}\tilde{x}_n^{(1)} \\
 x_{n-2} &= x_n - \frac{3}{2}x_n^{(1)} + \frac{1}{2}x_n^{(2)} - \frac{1}{2}\tilde{x}_n^{(2)} \\
 x_{n-3} &= x_n - \frac{3}{2}x_n^{(1)} + \frac{4}{2}x_n^{(2)} - \frac{1}{2}x_n^{(3)} + \frac{1}{2}\tilde{x}_n^{(3)}
 \end{aligned}$$

$$\begin{aligned}
 x_{n-4} &= x_n - \frac{5}{2}x_n^{(1)} + \frac{4}{2}x_n^{(2)} - \frac{5}{2}x_n^{(3)} + \frac{1}{2}x_n^{(4)} - \frac{1}{2}\tilde{x}_n^{(4)} \\
 x_{n-5} &= x_n - \frac{5}{2}x_n^{(1)} + \frac{9}{2}x_n^{(2)} - \frac{5}{2}x_n^{(3)} + \frac{6}{2}x_n^{(4)} - \frac{1}{2}x_n^{(5)} + \frac{1}{2}\tilde{x}_n^{(5)}
 \end{aligned}$$

which are useful to play with in order to understand in a concrete way the relations that follow.

The a_p^j are the coefficients to be computed but only some of them are needed, as indeed we consider differences $\Delta_p^k x_n$. For the definitions

$$\alpha_q^\ell = 2a_{2q+1}^{2\ell+1} \quad \beta_r^\ell = 2a_{2r}^{2\ell} \tag{A.5}$$

the first and second derivatives read ($p = 2q + 1$)

$$x_{n+p} - x_{n-p} = \sum_{\ell=0}^q \alpha_q^\ell \nabla^{2\ell+1} x_n \tag{A.6}$$

$$x_{n+2r} - 2x_n + x_{n-2r} = \sum_{\ell=1}^r \beta_r^\ell \nabla^{2\ell} x_n \tag{A.7}$$

and we prove hereafter the expressions (3.8) and (3.9) for the coefficients α_q^ℓ and β_r^ℓ [20]:

$$\alpha_q^\ell = \frac{(2q+1)(q+\ell)!}{(q-\ell)!(2\ell+1)!} \quad \beta_r^\ell = \frac{2r(r+\ell-1)!}{(r-\ell)!(2\ell)!} \tag{A.8}$$

Note that in (3.9) we simply have set $\gamma_q^\ell = \beta_r^\ell$ for $r = 2q + 1$.

As the point n is fixed (arbitrary), lighter notation can be used, namely

$$\begin{aligned}
 G_q &= x_n^{(2q+1)} & A_q &= x_{n+(2q+1)} - x_{n-(2q+1)} \\
 H_r &= x_n^{(2r)} & S_0 &= x_n & S_r &= x_{n+2r} + x_{n-2r}
 \end{aligned} \tag{A.9}$$

and the definition (A.1) can now be written as

$$G_q = \sum_{k=0}^q (-)^{q-k} C_{2q+1}^{q-k} A_k \quad H_r = \sum_{k=0}^r (-)^{r-k} C_{2r}^{r-k} S_k \tag{A.10}$$

while (A.6) and (A.7) become respectively (note that $\beta_r^0 = 2$)

$$A_q = \sum_{\ell=0}^q \alpha_q^\ell G_\ell \quad S_r = \sum_{\ell=0}^r \beta_r^\ell H_r \tag{A.11}$$

Note that neither in A_q nor in S_r do the tilde-differences (A.4) appear.

The first step is the computation of the coefficients α_q^ℓ . By replacing (A.10) in (A.11), we arrive at the following equivalent relations

$$A_q = \sum_{\ell=0}^q \alpha_q^\ell \sum_{k=0}^{\ell} (-)^{\ell-k} C_{2\ell+1}^{\ell-k} A_k \tag{A.12}$$

$$G_q = \sum_{k=0}^q (-)^{q-k} C_{2q+1}^{q-k} \sum_{\ell=0}^k \alpha_k^\ell G_\ell \tag{A.13}$$

which are *identities* valid for any function x_n , that is for any choice of the sequences $\{A_k\}$ and $\{G_\ell\}$. Consequently, the coefficients of each A_k and G_k identically vanish, which furnishes the equivalent recursion relations

$$\forall \{\ell, q\}, \quad \ell < q, \quad \sum_{k=\ell}^q (-)^{k-\ell} C_{2k+1}^{k-\ell} \alpha_q^k = 0 \quad \alpha_q^q = 1 \tag{A.14}$$

$$\forall \{\ell, q\}, \quad \ell < q, \quad \sum_{k=\ell}^q (-)^{q-k} C_{2q+1}^{q-k} \alpha_k^\ell = 0 \quad \alpha_q^q = 1. \tag{A.15}$$

The rest of the proof is the check that the expression of α_q^k given in (A.8) does solve the above recursion relations. This is easily done with help of the following identity

$$\sum_{m=0}^n (-1)^m \frac{(s+n+m-1)!}{m!(n-m)!(s+m)!} = 0 \quad (\text{A.16})$$

which can be obtained by differentiating n times a conveniently chosen polynomial of degree $n-1$ in the variable s , namely

$$Df(s) = f(s+1) - f(s) \quad D^n f(s) = \sum_{m=0}^n (-1)^{n-m} C_n^m f(s+m) \quad (\text{A.17})$$

$$f(s) = \frac{(s+n-2)!}{(s-1)!} \Rightarrow D^n f(s) = 0. \quad (\text{A.18})$$

The same procedure is then applied to obtain the coefficients β_q^k as given in (A.8).

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