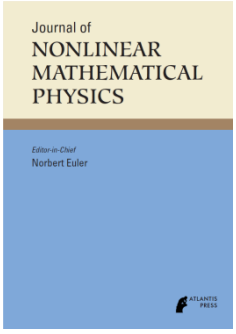

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DISCRETE MULTISCALE ANALYSIS: A BIATOMIC LATTICE SYSTEM

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We discuss a discrete approach to the multiscale reductive perturbative method and apply it to a biatomic chain with a nonlinear interaction between the atoms. This system is important to describe the time evolution of localized solitonic excitations.

We require that also the reduced equation be discrete. To do so coherently we need to discretize the time variable to be able to get asymptotic discrete waves and carry out a discrete multiscale expansion around them. Our resulting nonlinear equation will be a kind of discrete Nonlinear Schrödinger equation. If we make its continuum limit, we obtain the standard Nonlinear Schrödinger differential equation.

Keywords: Multiple scale expansions; asymptotic analysis on the lattice; integrable equations; nonlinear chains; discrete Nonlinear Schrödinger equation; biatomic lattices.

1. Introduction

Nonlinear systems, and in particular nonlinear discrete systems, are gaining an increasing impact in modern science [33].

In 1955 Fermi, Pasta and Ulam (FPU) [14] considered a unidimensional chain of atoms with nonlinear nearest neighboring interaction to verify if nonlinearity could produce energy equipartition. Instead, they found recurrence, i.e. the motion of the chain for small energies was almost periodic [43]. To explain this result Kruskal and Zabusky found in 1965 [42] a connection between the FPU system and the Korteweg–De Vries equation (KdV), an equation introduced in fluid dynamics to describe one dimensional surface waves in the shallow water context [20]. By introducing the Inverse Scattering Transform, they were able to solve the Cauchy problem for the KdV equation [15] and to prove the existence of soliton solutions.

In 1967 Toda [37] considered a dynamical system with exponential interaction, $U(r) = e^{-r} + r - 1$, the "Toda potential", whose small amplitude approximation gives the FPU system, and shares many of the integrability properties of the KdV equation. So the FPU system turns out to be an approximation of a discrete soliton model.

Later more complicate atomic chains have been considered, as, for example, the biatomic one [6, 9, 11, 12, 16, 26]. These systems have various applications in physics and biology as, for example, in the study of ferroelectric perovskites, materials that, in certain crystallographic directions have an almost unidimensional frame, and in organic molecular chains. A biatomic chain of neighboring atoms A_1 and A_2 is described by the discrete independent variable n and a continuous time t. However, the simplest nonlinear coupled lattice dynamical equations one can construct for this system are not solvable. Only special exact solutions may be found.

Multiscale expansions [7, 8, 19–21, 35, 36] have proved to be important tools to find approximate solutions for many physical problems by reducing a given nonlinear partial differential equation to a simpler equation, which is often integrable [5]. Recently, few attempts to carry over this approach to partial difference equations have been proposed [2, 10, 22, 23, 32]. Almost all approaches considered contain some approximation, either based on physical or on mathematical reasoning as scaling transformations of the lattice provide a nonlocal result. In the following we prefer to stick to mathematical approximations as in this case it will be more evident what to do to improve the final result [17].

In [9] a biatomic chain obtained as a first nonlinear approximation of a complex Lenard–Jones interaction between atoms has been considered. There the multiscale expansion of the continuous limit of the lattice model showed that the modulation of periodic solutions is governed by the Nonlinear Schrödinger differential Equation (NLSE). Here we consider the same model but we are interested in carrying out the multiscale expansion on the lattice, i.e. we are looking for a lattice equation which in the asymptotic regime approximate the biatomic nonlinear lattice. To do so we need to discretize time to be able to allow for discrete asymptotic waves. If we keep a continuous time variable an asymptotic wave travelling on the lattice by necessity will be described by a continuous variable. So by necessity we go over to a differential system.

Discretization of variables, besides representing an interesting problem in mathematical physics for its computerizability, it is also useful in itself. Measurements, for example, are based on sampling of physical variables such as space and time. It follows that physical models in which variables are defined on the lattice are easier to be compared with the real world we see in our measurements.

In this work, we propose to continue the previous researches of biatomic chains considering both t and n as discrete variables. In particular, we shall assume, as these authors, that the system has an unharmonic cubic potential as in nature, potentials usually are non–symmetric. We shall thus apply a discrete multiscale reductive perturbative method to the model introduced by Campa *et. al.* [9] consisting of a biatomic chain with a nonlinear nearest neighbor interaction.

In Sec. 2, we describe in detail the biatomic chain and write down the dynamical equations. Then in Sec. 3, we introduce some notions of discrete calculus and multiple scales defined on the lattice which we apply in Sec. 4 to the biatomic chain introduced in Sec. 2.

In Sec. 5, we analyze the resulting nonlinear discrete equation obtained and carry out its continuum limit. Finally, in Sec. 6, we draw some final conclusions.

2. The Model

We want to describe here a chain suitable to represent, for example, an α-helix channel, see Scott (1999) [33]. Our model consists of a biatomic chain formed by a sequence of pairs of neighboring atoms A_1 and A_2, with masses M_1 and M_2, respectively. Each pair, made of an atom of mass M_1 and the following one of mass M_2, can be considered as a "molecule". We denote by the index n the nth molecule formed by the atom A_1 and A_2 (see Fig. 1). Let us indicate with $x_n(t)$ and $y_n(t)$ the displacements of the atoms A_1 and A_2 belonging to the same molecule n. For each atom, we assume only nearest neighboring interactions. Then, the total potential of the chain is given by

$$U = \sum_n \{U_1(y_n - x_n) + U_2(x_{n+1} - y_n)\}, \tag{1}$$

where U_1 is the intramolecular potential, between atoms belonging to the same molecule, and U_2 is the potential between different molecules.

Given a natural [3, 6, 38] asymmetric potential with an absolute minimum in the equilibrium position as, for example, a Lenard–Jones potential, by taking the first terms of its Taylor expansion around the equilibrium position we can write the potentials U_1 and U_2 as

$$U_1(r) = \frac{1}{2}k_1 r^2 + \frac{\epsilon}{3}\beta_1 r^3, \quad U_2(r) = \frac{1}{2}k_2 r^2 + \frac{\epsilon}{3}\beta_2 r^3,$$

where k_1 and k_2 are the harmonic constants, β_1 and β_2 are the cubic interaction constants and ϵ is a small parameter which will play the role of the perturbative parameter. We assume that the interaction between atoms of the same site is stronger than that of atoms of different sites; thus $k_1 > k_2$ and $|\beta_1| > |\beta_2|$. So, the Hamiltonian of our molecular chain turns out to be

$$\begin{aligned} H = \sum_n \Bigg\{ & \frac{1}{2}[M_1 \dot{x}_n^2 + M_2 \dot{y}_n^2] + \frac{1}{2}[k_1(y_n - x_n)^2 + k_2(x_{n+1} - y_n)^2] \\ & + \frac{\epsilon}{3}[\beta_1(y_n - x_n)^3 + \beta_2(x_{n+1} - y_n)^3] \Bigg\}, \end{aligned}$$

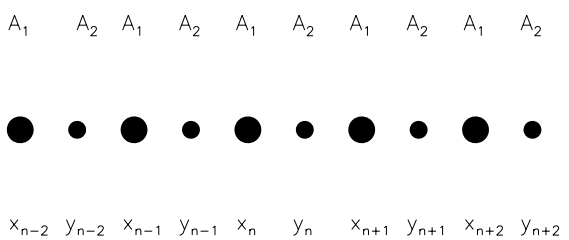

Fig. 1. Pattern of a biatomic molecular chain in one dimension. The chain is formed by a sequence of pairs of neighboring atoms A_1 and A_2. The displacements of the atoms of the molecule n are indicated with x_n and y_n.

where $\dot{x}(t) \equiv \frac{\mathrm{d}x(t)}{\mathrm{d}t}$ and the equations of motion are

$$\begin{aligned} M_1\ddot{x}_n &= -\frac{\partial H}{\partial x_n} \\ &= k_1(y_n - x_n) - k_2(x_n - y_{n-1}) + \epsilon\beta_1(y_n - x_n)^2 - \epsilon\beta_2(x_n - y_{n-1})^2, \qquad (2) \\ M_2\ddot{y}_n &= \frac{\partial H}{\partial y_n} \\ &= -k_1(y_n - x_n) + k_2(x_{n+1} - y_n) - \epsilon\beta_1(y_n - x_n)^2 + \epsilon\beta_2(x_{n+1} - y_n)^2. \qquad (3) \end{aligned}$$

Equations (2) and (3) are a natural extension of the FPU model [14] to a biatomic system.

3. Multiple Scales on a Lattice

Here we introduce the concepts necessary to extend the multiscale reductive perturbative approach introduced by Poincaré [5] for the study of the asymptotic expansion of ordinary differential equations and extended by Taniuti to the reduction of partial differential equations [35, 36] to the case of difference equations [17, 24, 32].

3.1. *Lattices and functions defined on them*

Given a lattice, we will denote by n the running index of the points separated by a constant spacing h. Thus to the lattice **index** n, we can associate a **continuous variable** $x = nh$ defining the position of the points with respect to the origin, for convenience chosen to be with no loss of generality $x_0 = 0$.

If we introduce a small parameter $\epsilon = N^{-1}$, where N is a large integer positive number, we can define on the same lattice the slowly varying discrete variables $n_j (j = 1, 2, 3, \ldots)$ of constant spacing H_j and the continuous variables x_j (see Fig. 2) where

$$n = N^j n_j, \quad x_j = \epsilon^j x. \qquad (4)$$

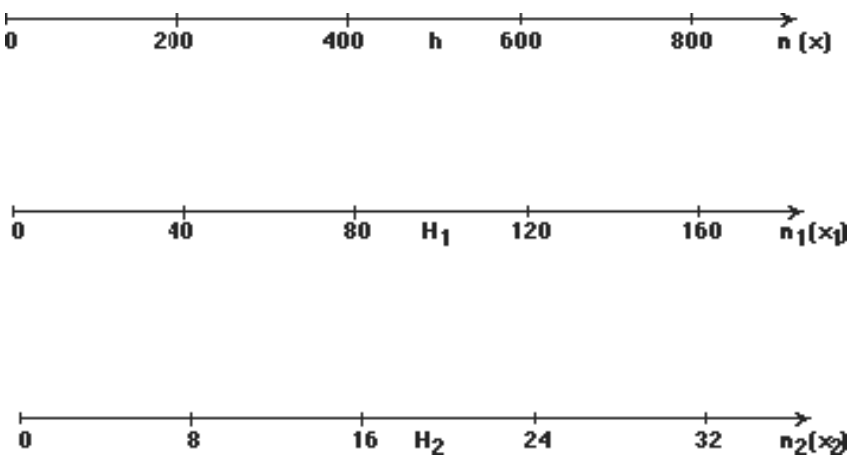

Fig. 2. Rescaled lattices.

If n_j varies by one, n varies by N^j, a number much larger than unity. For this reason, n_j is a "slow variable" and provide an asymptotic behavior of the system. For each j there is a slow lattice variable corresponding to the slow index n_j. n_j will be an integer only if n is a common multiple of N^j.

Let us consider F_n, a function of the discrete index n. An equation on the lattice is a functional relation which involves the function F at various lattice points, $\{F_{n+\ell}\}$. In the case of the model considered before (2, 3), $\ell = \pm 1$. We are interested to transform the system, defined on a lattice n, to the slowly varying lattices n_j, providing the scales of the asymptotic behavior of the original system. This is equivalent to say that we are interested in transforming the system defined on x to the one with the slowly varying variables x_j. We can consider the function F_n written in terms of the slowly varying lattice variables $\{n_j\}$, with, for example, $j = 1, 2, F_n \equiv f_{n_1,n_2}$, and we can carry out the ϵ expansion of the function $F_{n+\ell}$.

Let us consider at the beginning the case of one slowly varying lattice n_1, i.e. $F_n \equiv f_{n_1}$. As the shift operator T_n acting on F_n gives $T_n F_n = F_{n+1}$, we have $F_{n+\ell} = T_n^\ell F_n$. In order to extract the behavior of the function $F_{n+1} = F(x+h)$ on the new scales, let us carry out the Taylor expansion of F_{n+1} in powers of h. In such a case the shift operator can be expressed as an infinite order differential operator with respect to x, i.e.

$$T_n = \exp(h\partial_x) = \sum_{k=0}^{\infty} \frac{(h\partial_x)^k}{k!}. \tag{5}$$

Moreover, if we define a Δ operator as $\Delta_n^{(+)} \equiv (T_n - 1)/h$, we have

$$\partial_x = \frac{\log(1 + h\Delta_n^{(+)})}{h}, \tag{6}$$

and Eq. (5) could be written as

$$T_n = \sum_{k=0}^{\infty} \frac{(\log(1 + h\Delta_n^{(+)}))^k}{k!}. \tag{7}$$

Formulas (6) and (7) are written in terms of $\Delta_n^{(+)}$. However on the lattice we can define an infinite number of different difference operators which in the continuum limit, when h goes to zero, go over to the first order derivative. Among them it is important, as it is self-adjoint, the symmetric shift operators $\Delta_n^{(s)} \equiv \frac{1}{2h}(T_n - T_n^{-1})$. In this case we have

$$\partial_x = \frac{\operatorname{arcsinh}(h\Delta_n^{(s)})}{h}, \quad \rightarrow \quad T_n = \sum_{k=0}^{\infty} \frac{(\operatorname{arcsinh}(h\Delta_n^{(s)}))^k}{k!}. \tag{8}$$

Introducing the slowly varying variable x_1 and the corresponding lattice n_1 in Eq. (5), as $\partial_x = \epsilon\partial_{x_1}$, we have

$$T_n^\ell = e^{\ell h\partial_x} = e^{\ell\epsilon h\partial_{x_1}} = T_{n_1}^{\ell\epsilon} = \sum_{k=0}^{\infty} \frac{(\ell h\epsilon\partial_{x_1})^k}{k!}. \tag{9}$$

If we introduce more lattice variables, for example $\{n_j\}$, with $j = 1, 2$, then T_n becomes

$$T_n^\ell = T_{n_1}^{\ell\epsilon} T_{n_2}^{\ell\epsilon^2} = \sum_{k=0}^{\infty} \frac{(\ell\epsilon h\partial_{x_1})^k}{k!} \sum_{j=0}^{\infty} \frac{(\ell\epsilon^2 h\partial_{x_2})^j}{j!}. \tag{10}$$

Once we expand the operator ∂_{x_j} in terms of shift operators we get an expression for $F(n\pm\ell)$ in terms of variations of $f(n_1, n_2)$ with coefficients depending on ϵ and ℓ.

As delta operators are linear combinations of shift operators, from Eq. (13) it can be proved [18, 24] that for $\Delta = \Delta^{(+)}$ we have the following formula

$$(\Delta_{n_1}^{(+)})^k f_{n_1} = \sum_{i=k}^{\infty} \frac{k!}{i!} P(i,k) (\Delta_n^{(+)})^i F_n, \tag{11}$$

where $(\Delta_{n_1}^{(+)})^k f_{n_1}$ is the kth-difference of f_{n_1} respect to n_1, and the coefficients $P(i,k)$ are given by $P(i,j) = \sum_{\alpha=j}^{i} w^\alpha S_i^\alpha G_\alpha^j$, where ω is the ratio of the increment in the lattice of variable n with respect to that of variable n_1. In this case, taking into account Eq. (4), $\omega = N$. The coefficients S_i^α and G_α^j are the Stirling coefficients of the first kind and second kind, respectively. The result (11) can be inverted, providing:

$$(\Delta_n^{(+)})^k F_n = \sum_{i=k}^{\infty} \frac{k!}{i!} Q(i,k) (\Delta_{n_1}^{(+)})^i f_{n_1}, \tag{12}$$

where $Q(i,j)$ is the same as $P(i,j)$, but with $w = N^{-1} = \epsilon$.

A general way to get these formulas is provided by the *finite operator calculus* [13, 29, 30]. The finite operator calculus prescribes the following formula [25]

$$T_n^j = \sum_{k=0}^{\infty} \frac{(\epsilon)^k p_k(j)}{k!} (\Delta_{n_1})^k, \tag{13}$$

where the functions $p_k(j)$ are the unique basic sequence associated to the operator Δ_{n_1}, i.e. such that they satisfy the following conditions

$$\begin{gathered} p_0(n_1) = 1, \quad p_k(0) = 0 \quad \text{for all } k > 0, \\ \Delta_{n_1} p_k(n_1) = k p_{k-1}(n_1). \end{gathered} \tag{14}$$

The basic sequences can be directly obtained by the transfer formulae:

$$p_k(n_1) = n_1 \left(\frac{\Delta_{n_1}}{h\partial_{x_1}} \right)^{-k} {n_1}^{k-1}. \tag{15}$$

When $\Delta_{n_1} = \Delta_{n_1}^{(+)}$ or $\Delta_{n_1} = \Delta_{n_1}^{(s)}$, the basic sequences are:

$$\begin{aligned} p_k^{(+)}(n_1) &= h^k n_1 \left(\frac{e^{h\partial_{x_1}} - 1}{h\partial_{x_1}} \right)^{-k} {n_1}^{k-1} = (x_1)_k \equiv x_1(x_1 - h)\cdots(x_1 - kh + h), \\ p_k^{(s)}(n_1) &= h^k n_1 \left(\frac{e^{h\partial_{x_1}} - e^{-h\partial_{x_1}}}{2h\partial_{x_1}} \right)^{-k} {n_1}^{k-1} = 2^k G_k(x_1; -h, 2h), \end{aligned} \tag{16}$$

where $G_k(y;a,b)$ are the Gould polynomials [29] given by

$$\begin{aligned} G_k(y;a,b) &\equiv \frac{y}{y-ka}\left(\frac{y-ka}{b}\right)_k \\ &= \frac{y}{(y-ka)(b)^k}(y-ka)(y-ka-b)\cdots(y-ka-(k-1)b). \end{aligned} \tag{17}$$

Let us also mention that for each Δ_{n_1} operator we can write from Eq. (13)

$$(\partial_{x_1})^j = \frac{1}{h^j}\sum_{k=0}^{\infty}\frac{1}{k!}\left[\frac{\mathrm{d}^j}{\mathrm{d}y^j}p_k(y)\right]\Bigg|_{y=0}(\Delta_{n_1})^k, \tag{18}$$

i.e. we can express the partial derivative as an infinite sum of differences whose coefficients depends from the type of difference we are expanding into. In terms of $\Delta^{(+)}$, from Eqs. (13) and (16), Eq. (9) reads

$$T_n^\ell F_n = \sum_{k=0}^{\infty}\frac{(h\epsilon)^k(\ell)_k}{k!}(\Delta_{n_1}^{(+)})^k f_{n_1}, \tag{19}$$

while, in the symmetric difference case, it reads

$$T_n^\ell F_n = \sum_{k=0}^{\infty}\frac{(2h\epsilon)^k}{k!}G_k(l;-1,2)(\Delta_{n_1}^{(s)})^k f_{n_1}. \tag{20}$$

From Eqs. (19) and (20) we get that any finite shift in the original equation will give rise to an expression in the slowly varying variables which involves an infinity of lattice points or, equivalently, contains differences at all orders of the function f_{n_1}. So to get a reduced equation on a finite number of points we need to cut the series by requiring that the function f_{n_1} be of finite order of variation. Let us introduce the following definition:

Definition. The function f_n is a slow varying function of order p if

$$\Delta^{p+1}f_n = 0. \tag{21}$$

Then we can prove the following Theorem:

Theorem. *The function F_n is a slow varying function of order p iff f_{n_1} is a slowly varying function of order p in its own variable*, i.e. *if* $\Delta_{n_1}^{p+1}f_{n_1} = 0$.

Proof. The proof of this theorem will be given in the case of $\Delta = \Delta^+$, but it is easy to see that it is valid for any delta operator. It is divided into two parts:

(a) Let f_{n_1} be a slowly varying function of order p. From formula (12) it follows that

$$\Delta_n^{p+1}F_n = \sum_{i=p+1}^{\infty}\frac{(p+1)!}{i!}Q(i,p+1)\Delta_{n_1}^i f_{n_1} = 0, \tag{22}$$

i.e. F_n is also a slow function of order p.

(b) Let F_n be a slowly varying function of order p. From formula (11) it follows that

$$\Delta_{n_1}^{p+1} f_{n_1} = \sum_{i=p+1}^{\infty} \frac{(p+1)!}{i!} P(i, p+1) \Delta_n^i F_n = 0, \tag{23}$$

i.e. f_{n_1} is also a slow function of order p. □

The expansion (20) can be performed in two steps: at first we write the shift operator in the n variable in terms of the derivatives with respect to x_1 by formula (9) and then we expand the derivatives with respect to x_1 in term of delta operators by formula (18). In doing so we will have formulas in derivatives which are valid for any delta operator. Moreover the first expansion has ϵ dependent coefficients while the second will provide a finite number of terms only if we use the slow varying condition for the functions f_{n_1,n_2}.

Let us now explicitate the first terms of Eq. (20) for future use, at first in terms of the derivatives and then in delta operators assuming that the function f_{n_1,n_2} is a slow function at most of order 2. At first we shall consider the case in which we have only one slow lattice, just the variable n_1 is present and then we extend the result to the case of two slow lattices, n_1 and n_2 and to partial lattices n and m.

3.1.1. $F_n = f_{n_1} = f(x_1)$

From Eq. (9) we get

$$F_{n\pm1} = f_{(x_1)} \pm h\epsilon \partial_{x_1} f(x_1) + \frac{h\epsilon^2}{2!} \partial_{x_1}^2 f(x_1) + \mathcal{O}(\epsilon^3). \tag{24}$$

As from Eq. (18) for $p = 2$, $\partial_{x_1} = \Delta_{n_1}$ and $\partial^2{}_{x_1} = (\Delta_{n_1})^2$, then Eq. (24) reads

$$F_{n\pm1} = f_{n_1} \pm \frac{1}{2N}(f_{n_1+1} - f_{n_1-1}) + \frac{1}{2N^2}(f_{n_1+1} - 2f_{n_1} + f_{n_1-1}) + O(N^{-3}). \tag{25}$$

3.1.2. $F_n = f_{n_1,n_2} = f(x_1, x_2)$

$p = 2$ is the lowest nontrivial value of p for which we can consider F_n as a function of the two scales, n_1 and n_2. Taking $l = 1$, from Eq. (10) we have

$$\begin{aligned} F_{n\pm1} = f(x_1, x_2) &\pm h\epsilon \frac{\partial f(x_1, x_2)}{\partial x_1} + \frac{h^2\epsilon^2}{2} \frac{\partial^2 f(x_1, x_2)}{\partial x_1^2} \pm h\epsilon^2 \frac{\partial f(x_1, x_2)}{\partial x_2} \\ &+ h^2\epsilon^3 \frac{\partial}{\partial x_1} \frac{\partial f(x_1, x_2)}{\partial x_2} + O(\epsilon^4). \end{aligned} \tag{26}$$

If F_n is a slowly varying function of order two in n_1, it might be of order one in n_2. In this case, Eq. (26) becomes

$$F_{n\pm1} = f(x_1, x_2) \pm h\epsilon \frac{\partial f(x_1, x_2)}{\partial x_1} + \frac{h^2\epsilon^2}{2} \frac{\partial^2 f(x_1, x_2)}{\partial x_1^2} \pm h\epsilon^2 \frac{\partial f(x_1, x_2)}{\partial x_2} + O(\epsilon^3). \tag{27}$$

Moreover, from Eq. (18) it follows that $\partial_{x_2} = \Delta_{n_2}, \partial^2_{x_1} = (\Delta_{n_1})^2$ and $\partial_{x_1}\partial_{x_2} = \Delta_{n_1}\Delta_{n_2}$. Then Eqs. (26) and (27), written in terms of differences instead of derivatives, are given by

$$\begin{aligned} F_{n\pm1} = f_{n_1,n_2} &\pm \frac{1}{2N}(f_{n_1+1,n_2} - f_{n_1-1,n_2}) \\ &+ \frac{1}{2N^2}(f_{n_1+1,n_2} - 2f_{n_1,n_2} + f_{n_1-1,n_2}) \pm \frac{1}{2N^2}(f_{n_1,n_2+1} - f_{n_1,n_2-1}) \\ &+ \frac{1}{4N^3}(f_{n_1+1,n_2+1} - f_{n_1-1,n_2+1} - f_{n_1+1,n_2-1} + f_{n_1-1,n_2-1}) + O(N^{-4}) \end{aligned} \tag{28}$$

and

$$\begin{aligned} F_{n\pm1} = f_{n_1,n_2} &\pm \frac{1}{2N}(f_{n_1+1,n_2} - f_{n_1-1,n_2}) \\ &+ \frac{1}{2N^2}(f_{n_1+1,n_2} - 2f_{n_1,n_2} + f_{n_1-1,n_2}) \\ &\pm \frac{1}{2N^2}(f_{n_1,n_2+1} - f_{n_1,n_2-1}) + O(N^{-3}), \end{aligned} \tag{29}$$

respectively.

3.1.3. $F_{n,m} = f_{n_1,m_1,m_2} = f(x_1,t_1,t_2)$

In this case we have

$$\begin{aligned} F_{n,m\pm1} = f(x_1,t_1,t_2) &\pm \tau\epsilon\frac{\partial f(x_1,t_1,t_2)}{\partial t_1} \\ &+ \frac{\tau^2\epsilon^2}{2}\frac{\partial^2 f(x_1,t_1,t_2)}{\partial t_1^2} \pm \tau\epsilon^2\frac{\partial f(x_1,t_1,t_2)}{\partial t_2} + O(\epsilon^3), \end{aligned} \tag{30}$$

and

$$F_{n\pm1,m} = f(x_1,t_1,t_2) \pm h\epsilon\frac{\partial f(x_1,t_1,t_2)}{\partial x_1} + \frac{h^2\epsilon^2}{2}\frac{\partial^2 f(x_1,t_1,t_2)}{\partial x_1^2} + O(\epsilon^3). \tag{31}$$

In terms of differences, the last two equations are given by

$$\begin{aligned} F_{n,m\pm1} = f_{n_1,m_1,m_2} &\pm \frac{1}{2N}(f_{n_1,m_1+1,m_2} - f_{n_1,m_1-1,m_2}) \\ &+ \frac{1}{2N^2}(f_{n_1,m_1+1,m_2} - 2f_{n_1,m_1,m_2} + f_{n_1,m_1-1,m_2}) \\ &\pm \frac{1}{2N^2}(f_{n_1,m_1,m_2+1} - f_{n_1,m_1,m_2-1}) + O(N^{-3}) \end{aligned} \tag{32}$$

and

$$\begin{aligned} F_{n\pm1,m} = f_{n_1,m_1,m_2} &\pm \frac{1}{2N}(f_{n_1+1,m_1,m_2} - f_{n_1-1,m_1,m_2}) \\ &+ \frac{1}{2N^2}(f_{n_1+1,m_1,m_2} - 2f_{n_1,m_1,m_2} + f_{n_1-1,m_1,m_2}) + O(N^{-3}). \end{aligned} \tag{33}$$

For future use we can further rescale the lattice with some extra parameter by defining $n_1 = \frac{L_1 n}{N}, m_1 = \frac{L_2 m}{N}$ e $m_2 = \frac{m}{N^2}$, where the order 1 parameters L_1 and L_2 are divisors of N

and N^2 respectively if we require that n_1 and n_2 be integer numbers. In this case, Eqs. (30) and (31) become

$$F_{n,m\pm1} = f(x_1,t_1,t_2) \pm \tau L_2 \epsilon \frac{\partial f(x_1,t_1,t_2)}{\partial t_1} + \frac{\tau^2 L_2^2 \epsilon^2}{2} \frac{\partial^2 f(x_1,t_1,t_2)}{\partial t_1^2} \pm \tau \epsilon^2 \frac{\partial f(x_1,t_1,t_2)}{\partial t_2} + O(\epsilon^3), \tag{34}$$

and

$$F_{n\pm1,m} = f(x_1,t_1,t_2) \pm h L_1 \epsilon \frac{\partial f(x_1,t_1,t_2)}{\partial x_1} + \frac{h^2 L_1^2 \epsilon^2}{2} \frac{\partial^2 f(x_1,t_1,t_2)}{\partial x_1^2} + O(\epsilon^3). \tag{35}$$

Moreover, from Eq. (34) we have

$$F_{n,m+1} - 2F_{n,m} + F_{n,m-1} = \tau^2 L_2^2 \epsilon^2 \frac{\partial^2 f(x_1,t_1,t_2)}{\partial t_1^2} + O(\epsilon^3). \tag{36}$$

In terms of symmetric difference operators these equations can be written as

$$\begin{aligned} F_{n,m\pm1} &= f_{n_1,m_1,m_2} \pm \frac{L_2}{2N}(f_{n_1,m_1+1,m_2} - f_{n_1,m_1-1,m_2}) \\ &\quad + \frac{L_2^2}{2N^2}(f_{n_1,m_1+1,m_2} - 2f_{n_1,m_1,m_2} + f_{n_1,m_1-1,m_2}) \\ &\quad \pm \frac{1}{2N^2}(f_{n_1,m_1,m_2+1} - f_{n_1,m_1,m_2-1}) + O(N^{-3}), \end{aligned} \tag{37}$$

$$\begin{aligned} F_{n\pm1,m} &= f_{n_1,m_1,m_2} \pm \frac{L_1}{2N}(f_{n_1+1,m_1,m_2} - f_{n_1-1,m_1,m_2}) \\ &\quad + \frac{L_1^2}{2N^2}(f_{n_1+1,m_1,m_2} - 2f_{n_1,m_1,m_2} + f_{n_1-1,m_1,m_2}) + O(N^{-3}) \end{aligned} \tag{38}$$

and

$$\begin{aligned} F_{n,m+1} - 2F_{n,m} + F_{n,m-1} &= \frac{L_2^2}{N^2}(f_{n_1,m_1+1,m_2} - 2f_{n_1,m_1,m_2} + f_{n_1,m_1-1,m_2}) \\ &\quad + O(N^{-3}). \end{aligned} \tag{39}$$

The last three equations will be used in the following section to apply the multiscale method to the biatomic lattice model we introduced in Sec. 2.

4. Multiscale Reduction of the Discrete Biatomic System

4.1. *Equations of motion*

In the equations of motion of the biatomic chain (see Eqs. (2) and (3)), the nonlinear terms (proportional to β_1 and β_2) are of order ϵ respect to the remaining terms, and thus we can use perturbative methods to look for approximate solutions of $x_n(t)$ and $y_n(t)$. This has been done in 1993 by Campa *et al.* [9] using the multiscale perturbative method with just the lowest order differential terms. In this way, performing at the same time a multiscale expansion and a continuum limit they were able to reduce the system to the NLSE (69).

Here we discretize time and look for completely discrete equations, i.e. passing from the differential terms in the expansion (see Eqs. (24), (26), (27), (30), (31), (34)–(36)) to difference terms corresponding to the lowest order of slow varyness p, i.e. to Eqs. (25), (28), (29), (32), (33), (37)–(39). To discretize time we replace the time t with a discrete variable m, so that $t \equiv m\tau$, where τ is the temporal scale. Thus, when τ reduces to an infinitesimal quantity and m approaches infinity in such a way that t remains finite we recover the continuous case. We consider the simplest approximation of the second derivative by differences using a central difference so as to get a real dispersive relation. The discretized equations of motion are given by

$$\begin{aligned} m_1(x_{n,m+1} - 2x_{n,m} + x_{n,m-1}) &= k_1(y_{n,m} - x_{n,m}) - k_2(x_{n,m} - y_{n-1,m}) \\ &\quad + \epsilon[\beta_1(y_{n,m} - x_{n,m})^2 - \beta_2(x_{n,m} - y_{n-1,m})^2], \qquad (40) \\ m_2(y_{n,m+1} - 2y_{n,m} + y_{n,m-1}) &= -k_1(y_{n,m} - x_{n,m}) + k_2(x_{n+1,m} - y_{n,m}) \\ &\quad - \epsilon[\beta_1(y_{n,m} - x_{n,m})^2 - \beta_2(x_{n+1,m} - y_{n,m})^2], \qquad (41) \end{aligned}$$

where $x_{n,m} \equiv x_n(m\tau), y_{n,m} \equiv y_n(m\tau)$ and $m_{1,2} \equiv \frac{M_{1,2}}{\tau^2}$. We are looking for $x_{n,m}$ and $y_{n,m}$ as bounded solutions written as a modulation of the harmonic wave solutions of the linearized equations which one obtains when setting $\epsilon = 0$. The harmonic waves are given by

$$E_{n,m} = e^{i[kn - \omega(k)m]}, \qquad (42)$$

with $\omega(k)$ real for any real value of k. The physical reason for choosing harmonic waves is that the atoms of the chain make only small oscillations around their equilibrium position. When we introduce this ansatz into Eqs. (40) and (41), we realize at once that the solution of the nonlinear equations of motion can be represented as a modulated linear combination of harmonic functions.

A solution of the linear part of Eqs. (40) and (41) ($\beta_1 = \beta_2 = 0$), written in terms of the harmonic waves (42), is given by

$$x_{n,m} = AE_{n,m}, \quad y_{n,m} = BE_{n,m},$$

where

$$\frac{B}{A} = r \equiv \frac{k_1 + k_2 + 2m_1(\cos\omega(k) - 1)}{k_1 + k_2 e^{-ik}} = \frac{k_1 + k_2 e^{ik}}{k_1 + k_2 + 2m_2(\cos\omega(k) - 1)}, \qquad (43)$$

with the dispersion relation

$$\begin{aligned} \omega(k) = \arccos\Bigg\{ 1 - \frac{1}{4m_1m_2}\Bigg[&(k_1 + k_2)(m_1 + m_2) \\ &\pm \sqrt{(k_1 + k_2)^2(m_1 + m_2)^2 - 16k_1k_2m_1m_2 sin^2\frac{k}{2}} \Bigg]\Bigg\}. \qquad (44) \end{aligned}$$

It can be proved that the term inside the square root of the dispersion relation is always positive, so that the argument of "arccos" is always real.

In Eq. (44), the positive sign corresponds to the optical branch $\omega_{\text{opt}}(k)$, whereas the negative one to the acoustical branch $\omega_{\text{ac}}(k)$. It can be proved that the function $\omega(k)$ is real

for all real values of k iff the temporal scale τ satisfies the following inequalities:

$$\tau \leq \sqrt{\frac{4M_1M_2}{(k_1+k_2)(M_1+M_2)}} \equiv \tau_o \tag{45}$$

for the optical branch, and

$$\tau \leq \sqrt{\frac{8M_1M_2}{(k_1+k_2)(M_1+M_2)-\sqrt{(k_1+k_2)^2(M_1+M_2)^2-16k_1k_2M_1M_2}}} \equiv \tau_a \tag{46}$$

for the acoustical one. It is easy to show that τ_a is always larger than τ_o. In Figs. 3, 4 we show how $\omega(k)$ varies as a function of τ. We have chosen, following Campa [9], the following numerical values for the parameters, $M_1 = 1$, $M_2 = 1.5$, $k_1 = 1$ and $k_2 = 0.3$, so that $\tau_o \simeq 1.358732$ and $\tau_a \simeq 2.910816$. So the obtained threshold values τ_o and τ_a are consistent with the request that τ, the discretization parameter, be smaller than one.

Let us seek a finite amplitude solution of the nonlinear system (40), (41). To do so, we write $x_{n,m}$ and $y_{n,m}$ in terms of the harmonics of the linearized Eq. (42)

$$x_{n,m} = \sum_{s=0}^{\infty} G^s_{n,m}(E_{n,m})^s + \sum_{s=1}^{\infty} \bar{G}^s_{n,m}(E_{n,m})^{-s}, \tag{47}$$

$$y_{n,m} = \sum_{s=0}^{\infty} H^s_{n,m}(E_{n,m})^s + \sum_{s=1}^{\infty} \bar{H}^s_{n,m}(E_{n,m})^{-s}, \tag{48}$$

where, as the variables $x_{n,m}$ and $y_{n,m}$ are real, $(\bar{G}^s_{n,m}, \bar{H}^s_{n,m})$ are the complex conjugates of the modulation coefficients $(G^s_{n,m}, H^s_{n,m})$. We choose $G^s_{n,m} = g^s_{n_1,m_1,m_2}$ and $H^s_{n,m} = h^s_{n_1,m_1,m_2}$ as slowly varying functions of the second order in n_1 and m_1 and of the first order

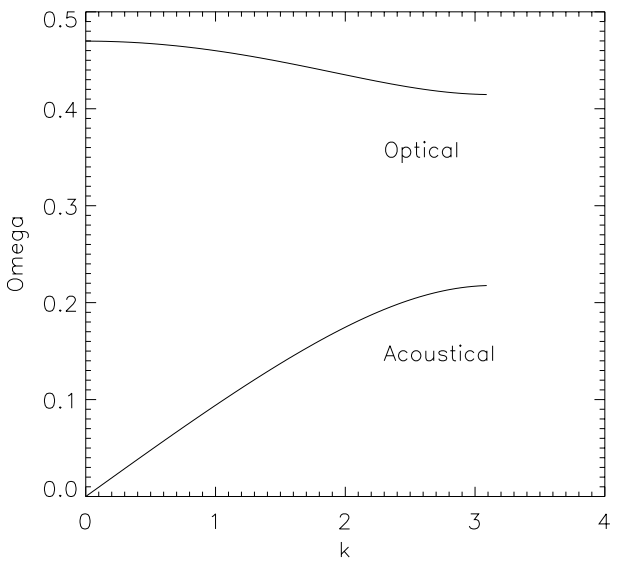

Fig. 3. Graph of $\omega(k)$ against k, with k lying in the interval $[0, \pi]$. We have chosen $M_1 = 1, M_2 = 1.5$, $k_1 = 1$, $k_2 = 0.3$ and $\tau = 10^{-1/2}$.

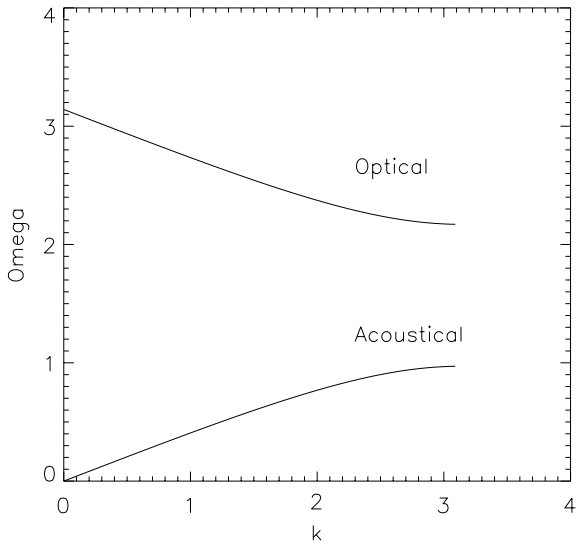

Fig. 4. Graph of $\omega(k)$ against k, with k lying in the interval $[0, \pi]$. The parameters M_1, M_2, k_1, and k_2 are the same as in Fig. 4, but $\tau = \tau_o$.

in m_2, defined in such a way to avoid secular terms. Moreover we expand the functions $g^s_{n_1,m_1,m_2}$ and $h^s_{n_1,m_1,m_2}$ in the small parameter ϵ. So we have:

$$G^s_{n,m} \equiv \sum_{l=0}^{\infty} \epsilon^l g^{(s,l)}_{n_1,m_1,m_2}, \tag{49}$$

$$H^s_{n,m} \equiv \sum_{l=0}^{\infty} \epsilon^l h^{(s,l)}_{n_1,m_1,m_2}. \tag{50}$$

4.2. *Derivation of the equations of motion*

Substituting ansatz (47), (48) into the equations of motion (40), (41) and taking into account Eqs. (49) and (50) we get two equations of the form

$$\sum_{s=0}^{\infty}\sum_{l=0}^{\infty} \epsilon^l F^{(s,l)}_{n_1,m_1,m_2}(E_{n,m})^s + \sum_{s=0}^{\infty}\sum_{l=0}^{\infty} \epsilon^l \bar{F}^{(s,l)}_{n_1,m_1,m_2}(E_{n,m})^{-s} = 0, \tag{51}$$

where the $F^{(s,l)}_{n_1,m_1,m_2}$ are function only of the slow variables. As $(E_{n,m})^s$ and $(E_{n,m})^{-s}$ are independent functions, its coefficients must be equal to zero. So for each power of $(E_{n,m})$ and ϵ we get sets of equations $F^{(s,l)}_{n_1,m_1,m_2} = 0$ for the slow varying modulation coefficients $g^{(s,l)}_{n_1,m_1,m_2}$ and $h^{(s,l)}_{n_1,m_1,m_2}$ together with their complex conjugate.

4.2.1. ϵ^0

We look here for the linearized terms. In this case, the coefficient of the zeroth harmonic satisfies the equation

$$g^{(0,0)}_{n_1,m_1,m_2} = h^{(0,0)}_{n_1,m_1,m_2}, \tag{52}$$

whereas the coefficients of the first harmonics gives a set of two equations that are identically satisfied when $\omega(k)$ satisfies the dispersion relation (44) and

$$\frac{h^{(1,0)}_{n_1,m_1,m_2}}{g^{(1,0)}_{n_1,m_1,m_2}} = r. \tag{53}$$

It can be proven easily that, for $q \geq 2, g^{(q,0)}_{n_1,m_1,m_2} = h^{(q,0)}_{n_1,m_1,m_2} = 0$.

4.2.2. ϵ^1

The coefficients of the zeroth harmonic are

$$h^{(0,1)}(x_1,t_1,t_2) = g^{(0,1)}(x_1,t_1,t_2) + \frac{hL_1k_2}{k_1+k_2}\frac{\partial g^{(0,0)}(x_1,t_1,t_2)}{\partial x_1} + \frac{2}{k_1+k_2}[\beta_2|1-e^{-ik}r|^2 - \beta_1|1-r|^2]|g^{(1,0)}(x_1,t_1,t_2)|^2, \tag{54}$$

or

$$h^{(0,1)}_{n_1,m_1,m_2} = g^{(0,1)}_{n_1,m_1,m_2} + \frac{L_1k_2}{2(k_1+k_2)}(g^{(0,0)}_{n_1+1,m_1,m_2} - g^{(0,0)}_{n_1-1,m_1,m_2}) + \frac{2}{k_1+k_2}[\beta_2|1-e^{-ik}r|^2 - \beta_1|1-r|^2]|g^{(1,0)}_{n_1,m_1,m_2}|^2, \tag{55}$$

depending if we use the expansions in terms of derivatives or differences.

For $s = 1$ we find a system of two equations in the two unknowns, $g^{(1,1)}_{n_1,m_1,m_2}$ and $h^{(1,1)}_{n_1,m_1,m_2}$. This system is compatible only if

$$g^{(1,0)}_{n_1,m_1,m_2} \equiv g^{(1,0)}_{n_2,m_2}, \tag{56}$$

where $n_2 = n_1 - m_1$ and

$$h^{(1,1)}_{n_1,m_1,m_2} = rg^{(1,1)}_{n_1,m_1,m_2} + \frac{2i\sin\omega m_1\omega_{,k} + k_2re^{-ik}}{2(k_1+k_2e^{-ik})}L_1(g^{(1,0)}_{n_2+1,m_2} - g^{(1,0)}_{n_2-1,m_2}), \tag{57}$$

where $\omega_{,k} \equiv \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{L_2}{L_1}$, with L_1 and L_2 given in Appendix A.1 by Eqs. (72) and (73). The differential version of Eq. (56) is

$$g^{(1,0)}(x_1,t_1,t_2) \equiv g^{(1,0)}(x_2,t_2),$$

where $x_2 \equiv hn_2 = h(n_1-m_1) = x_1 - \frac{h}{\tau}t_1$, and

$$h^{(1,1)}(x_1,t_1,t_2) = rg^{(1,1)}(x_1,t_1,t_2) + \frac{2i\sin\omega m_1\omega_{,k} + k_2re^{-ik}}{k_1+k_2e^{-ik}}hL_1\frac{\partial g(x_2,t_2)^{(1,0)}}{\partial x_2}. \tag{58}$$

For the second harmonic we get

$$g^{(2,1)}_{n_1,m_1,m_2} = K_1g^{(1,0)2}_{n_1,m_1,m_2}, \tag{59}$$

$$h^{(2,1)}_{n_1,m_1,m_2} = K_2g^{(1,0)2}_{n_1,m_1,m_2}, \tag{60}$$

where K_1 and K_2 are given in Appendix A.1 by Eqs. (75) and (76). It can be easily proven that, for $q \geq 3, g^{(q,1)}_{n_1,m_1,m_2} = h^{(q,1)}_{n_1,m_1,m_2} = 0$.

4.2.3. ϵ^2

Taking into account Eq. (56), the zeroth harmonic gives a system of two equations that is satisfied only if

$$L_1^2(g^{(0,0)}_{n_2+1,m_2} + g^{(0,0)}_{n_2-1,m_2} - 2g^{(0,0)}_{n_2,m_2}) = L_1\frac{c^0}{2}(|g^{(1,0)}_{n_2+1,m_2}|^2 - |g^{(1,0)}_{n_2-1,m_2}|^2)$$
$$+ L_1\frac{c^1}{2}\{g^{(1,0)}_{n_2,m_2}(\bar{g}^{(1,0)}_{n_2+1,m_2} - \bar{g}^{(1,0)}_{n_2-1,m_2}) + \bar{g}^{(1,0)}_{n_2,m_2}(g^{(1,0)}_{n_2+1,m_2} - g^{(1,0)}_{n_2-1,m_2})\}, \tag{61}$$

where c^0 and c^1 are two real constants given in Appendix A.3. Defining

$$A_{n_2,m_2} \equiv L_1(g^{(0,0)}_{n_2+1,m_2} - g^{(0,0)}_{n_2,m_2}) - \frac{c^0}{2}(|g^{(1,0)}_{n_2+1,m_2}|^2 + |g^{(1,0)}_{n_2,m_2}|^2)$$
$$- \frac{c^1}{2}(g^{(1,0)}_{n_2,m_2}\bar{g}^{(1,0)}_{n_2+1,m_2} + \bar{g}^{(1,0)}_{n_2,m_2}g^{(1,0)}_{n_2+1,m_2}), \tag{62}$$

Eq. (61) reads:

$$A_{n_2+1,m_2} - A_{n_2,m_2} = 0. \tag{63}$$

Thus $A_{n_2,m_2} = C(m_2)$, where $C(m_2)$ is an arbitrary function of m_2. Using the fact that $g^{(0,0)}_{n_2,m_2}$ is a slowly varying function in n_2 we have

$$L_1(g^{(0,0)}_{n_2+1,m_2} - g^{(0,0)}_{n_2-1,m_2}) = c^0(|g^{(1,0)}_{n_2+1,m_2}|^2 + |g^{(1,0)}_{n_2,m_2}|^2)$$
$$+ c^1(g^{(1,0)}_{n_2,m_2}\bar{g}^{(1,0)}_{n_2+1,m_2} + \bar{g}^{(1,0)}_{n_2,m_2}g^{(1,0)}_{n_2+1,m_2}) + C(m_2). \tag{64}$$

Equation (64) written in terms of the derivatives reads:

$$hL_1\frac{\partial g^{(0,0)}(x_2,t_2)}{\partial x_2} = (c^0 + c^1)|g^{(1,0)}_{n_2,m_2}|^2 + \frac{C(m_2)}{2}. \tag{65}$$

If we transform the derivatives of Eq. (65) into differences (using again Eq. (18), and recalling that $x_2 = hn_2$), we have

$$L_1(g^{(0,0)}_{n_2+1,m_2} - g^{(0,0)}_{n_2-1,m_2}) = 2(c^0 + c^1)|g^{(1,0)}_{n_2,m_2}|^2 + C(m_2), \tag{66}$$

an equation simpler than Eq. (64). This difference is due to the fact that Eq. (65) is obtained using the Leibniz's rule and an integration, while in the case of Eq. (64) the Leibniz's rule is not applicable as we deal with differences.

Finally, for $s = 1$, we get a system of two equations in the two unknowns, $g^{(1,2)}_{n_2,m_2}$ and $h^{(1,2)}_{n_2,m_2}$, which is compatible and not–secular only if

$$iB_1(g^{(1,0)}_{n_2,m_2+1} - g^{(1,0)}_{n_2,m_2-1}) + B_2L_1^2(g^{(1,0)}_{n_2+1,m_2} + g^{(1,0)}_{n_2-1,m_2} - 2g^{(1,0)}_{n_2,m_2})$$
$$+ B_3|g^{(1,0)}_{n_2,m_2}|^2g^{(1,0)}_{n_2,m_2} + \{B_4(|g^{(1,0)}_{n_2+1,m_2}|^2 + |g^{(1,0)}_{n_2,m_2}|^2) + B_5(g^{(1,0)}_{n_2,m_2}\bar{g}^{(1,0)}_{n_2+1,m_2}$$
$$+ \bar{g}^{(1,0)}_{n_2,m_2}g^{(1,0)}_{n_2+1,m_2}) + B_6C(m_2)\}g^{(1,0)}_{n_2,m_2} = 0. \tag{67}$$

Here the coefficients $B_i (i = 1, \ldots, 6)$ are real and given in Appendix A.3. This is a NLSE on the lattice. At difference from the standard discrete–time NLS equation presented by

Ablowitz and Ladik [1], this is completely local but not integrable [28, 39]. In the development of $x_{n,m}$ and $y_{n,m}$, $g^{(1,0)}_{n_2,m_2}$ is the main term which multiplies ϵ^0 and $E_{n,m}$. If we require that $g^{(s,l)}_{n_2,m_2}$ and $h^{(s,l)}_{n_2,m_2}$ are localized with respect to n_2, we have to set $C(m_2) = 0$ and Eq. (67) becomes

$$\begin{aligned} &iB_1(g^{(1,0)}_{n_2,m_2+1} - g^{(1,0)}_{n_2,m_2-1}) + B_2L_1^2(g^{(1,0)}_{n_2+1,m_2} + g^{(1,0)}_{n_2-1,m_2} - 2g^{(1,0)}_{n_2,m_2}) + B_3|g^{(1,0)}_{n_2,m_2}|^2 g^{(1,0)}_{n_2,m_2} \\ &\quad + \{B_4(|g^{(1,0)}_{n_2+1,m_2}|^2 + |g^{(1,0)}_{n_2,m_2}|^2) + B_5(g^{(1,0)}_{n_2,m_2}\bar{g}^{(1,0)}_{n_2+1,m_2} \\ &\quad + \bar{g}^{(1,0)}_{n_2,m_2}g^{(1,0)}_{n_2+1,m_2})\}g^{(1,0)}_{n_2,m_2} = 0. \end{aligned} \tag{68}$$

5. Continuum Limit of the Discrete NLS

Equation (68) is obtained from Eqs. (40) and (41) by discretizing the continuous time variable. This discretization was necessary to be able to solve the $l = 1, s = 1$ system which otherwise would have been an unsolvable linear differential difference wave equation. By discretizing we get a discrete wave equation whose general solution is given by an arbitrary function of a discrete variable.

It is interesting to perform the limit when the discrete time m_1 is transformed into a continuous t–variable. To do so, we take the limit when τ goes to zero and m tends to ∞ in such a way that the product $\tau m = t$ is finite. So Eq. (68) becomes the integrable NLSE

$$iA_1\frac{\partial g^{(1,0)}(z_2,t_2)}{\partial t_2} + A_2\frac{\partial^2 g^{(1,0)}(z_2,t_2)}{\partial {z_2}^2} + [A_3|g^{(1,0)}(z_2,t_2)|^2 + A_4C(t_2)]g^{(1,0)}(z_2,t_2) = 0, \tag{69}$$

where $t_2 = \lim_{\tau\to 0}\lim_{m\to\infty}\tau m_2$ and $z_2 = \frac{1}{N}(n_1 - \frac{\mathrm{d}\Omega}{\mathrm{d}k}t_1)$ is a new continuous variable. The coefficients $A_i (i = 1, \ldots, 4)$ in this limit are finite and real, and are given by

$$\begin{aligned} A_1 &= \lim_{\tau\to 0} 2\tau B_1 = -\Omega\frac{(M_1+M_2)(k_1+k_2) - 2M_1M_2\Omega^2}{k_1+k_2-M_2\Omega^2}, \\ A_2 &= \lim_{\tau\to 0} B_2 = \frac{[(M_1+M_2)(k_1+k_2) - 2M_1M_2\Omega^2)](\Omega_{,k})^2 - M_1M_2(\Omega_{,k})^2 - k_1k_2\cos k}{k_1+k_2-M_2\Omega^2}, \\ A_3 &= \lim_{\tau\to 0}(B_3 + 2B_4 + 2B_5) = \lim_{\tau\to 0}(B_3 + 2(c_0+c_1)B_6) \\ &= -2\beta_1^2(\bar{R}-1)\left\{(R-1)|R-1|^2\frac{2k_2(1-\cos k) - (M_1+M_2)\Omega^2}{D}\right. \\ &\quad \left. + \frac{2(R-1)}{k_1+k_2}|1-R|^2\right\} + 2\beta_2^2(1-\bar{R}e^{ik})\left\{-(1-Re^{-ik})\right. \\ &\quad \left.\times|1-Re^{-ik}|^2\frac{2k_1(1-\cos k) - (M_1+M_2)\Omega^2}{D} + \frac{2(Re^{-ik}-1)}{k_1+k_2}|1-Re^{-ik}|^2\right\} \\ &\quad + 2\beta_1\beta_2(\bar{R}-1)\left\{(\bar{R}-1)(1-Re^{-ik})^2\frac{(M_2+M_1e^{2ik})\Omega^2}{D} + \frac{2(R-1)}{k_1+k_2}|1-Re^{-ik}|^2\right\} \end{aligned}$$

$$+ 2\beta_1\beta_2(1-\bar{R}e^{ik})\left\{(R-1)^2(1-\bar{R}e^{ik})\frac{(M_2+M_1e^{-2ik})\Omega^2}{D}\right.$$

$$\left. + \frac{2(1-Re^{-ik})}{k_1+k_2}|1-R|^2\right\} + 2gA_4,$$

$$A_4 = \lim_{\tau\to 0} B_6 = \frac{k_1\beta_2|1-Re^{-ik}|^2 + k_2\beta_1|1-R|^2}{k_1+k_2},$$

where

$$g = \lim_{\tau\to 0}(c_1+c_2)\frac{2\beta_2 k_1|1-Re^{-ik}|^2 + 2\beta_1 k_2|1-R|^2}{(M_1+M_2)(k_1+k_2)(\Omega_{,k})^2 - k_1k_2},$$

$$D = [k_1+k_2-M_1\Omega^2][k_1+k_2-M_2\Omega^2] - (k_1^2+k_2^2+2k_1k_2\cos 2k), \tag{70}$$

and

$$R = \lim_{\tau\to 0} r = \frac{k_1+k_2-M_1\Omega^2}{k_1+k_2e^{-ik}}.$$

$\Omega(k) = \lim_{\tau\to 0}\frac{\omega(k)}{\tau}$ gives back the continuous dispersion relation [9].

6. Conclusions

In this work, introducing the concepts necessary for applying the perturbative multiscale method to discrete equations we have obtained a rescaled discrete equation. We have applied this technique to a biatomic chain model. In this way we have shown that we can perform in a coherent way a multiscale expansion on the lattice. If we want to remain on the lattice and want to avoid nonlocality then we need to restrict ourselves to slow–varying functions. This restriction on the class of function implies that some of the properties of the starting system will be lost. Among them by sure that of the integrability, which is strictly related to the analytic properties of the solutions.

We have found that $g^{(1,0)}$ (the slowly varying coefficient of the first harmonic) satisfies a totally discrete local version of the discrete NLSE. One interesting feature of our discrete NLSE is that, when we perform the continuous limit in the time variable, the spatial variable becomes continuous, and we get the continuous integrable NLSE (69) as in the work by Campa *et al.* [9].

A. Appendix

A.1. $g^{(1,1)}_{n_2,m_2}$ and $h^{(1,1)}_{n_2,m_2}$

Let us consider the expansion of the equations of motion with $l = s = 1$. In this case we get a system of two equations in two unknowns, $g^{(1,1)}_{n_1,m_1,m_2}$ and $h^{(1,1)}_{n_1,m_1,m_2}$, that is compatible only if

$$[(k_1+k_2)(m_1+m_2) + 4m_1m_2(\cos\omega - 1)]\sin(\omega)L_2(g^{(1,0)}_{n_1,m_1+1,m_2}$$
$$- g^{(1,0)}_{n_1,m_1-1,m_2}) + k_1k_2\sin kL_1(g^{(1,0)}_{n_1+1,m_1,m_2} - g^{(1,0)}_{n_1-1,m_1,m_2}) = 0. \tag{71}$$

It is convenient to choose

$$L_1 = S\sin(\omega)[(k_1+k_2)(m_1+m_2)+4m_1m_2(\cos\omega-1)] \tag{72}$$

and

$$L_2 = Sk_1k_2\sin k, \tag{73}$$

where S is a real number such that $L_1(L_2)$ is an integer number. In terms of L_1 and L_2 the dispersion relation becomes $\omega_{,k} = \frac{L_2}{L_1}$. With this choice of L_1 and L_2, and assuming that $g^{(1,0)}_{n_1,m_1,m_2} = g^{(1,0)}_{n_2,m_2}$, with $n_2 \equiv n_1 - m_1$, we find that Eq. (71) is satisfied. Thus the system of equations we are studying is compatible, and leads us to the Eq. (57).

A.2. *The discrete NLSE*

In this Appendix, we show the steps necessary to find the discrete NLSE (68). First, we take the equations of motion, and select the harmonic $s = 1$ with $l = 2$. In this way we get a system of two equations in the two unknowns $g^{(1,2)}_{n_2,m_2}$ and $h^{(1,2)}_{n_2,m_2}$, which is compatible only if the nonhomogeneous first order difference equation

$$\begin{aligned}&[(k_1+k_2)(m_1+m_2)+4m_1m_2(\cos\omega-1)]\sin(\omega)L_2(g^{(1,1)}_{n_1,m_1+1,m_2}\\&\quad - g^{(1,1)}_{n_1,m_1-1,m_2}) + k_1k_2\sin kL_1(g^{(1,1)}_{n_1+1,m_1,m_2} - g^{(1,1)}_{n_1-1,m_1,m_2})\\&= F(g^{(0,0)}_{n_2+1,m_2}, g^{(0,0)}_{n_2-1,m_2}, g^{(1,0)}_{n_2,m_2}),\end{aligned} \tag{74}$$

is satisfied. Here $F \equiv F(g^{(0,0)}_{n_2\pm1,m_2}, g^{(1,0)}_{n_2,m_2})$ is a given nonhomogeneous term. As the l.h.s. of this equation is the same as that of Eq. (71) (but with $g^{(1,1)}_{n_2\pm1,m_2}$ replaced by $g^{(1,0)}_{n_2\pm1,m_2}$), the terms depending on $g^{(1,0)}$ contained in F lead to secular terms for the unknown $g^{(1,1)}$. To avoid secular terms, we must set $F = 0$ and Eq. (74) gives $g^{(1,1)}_{n_1,m_1,m_2} = g^{(1,1)}_{n_2,m_2}$.

If we substitute $g^{(0,0)}$ given by Eq. (64) into $F = 0$, then this condition will give Eq. (68) written in terms of $g^{(1,0)}$.

A.3. *Constants*

We give here the expressions of the coefficients appearing in Eqs. (59), (60), (64) and (68):

(1) Eqs. (59) and (60).

$$\begin{aligned}K_1 \equiv\ &\{\beta_1(r-1)^2[k_1+k_2e^{ik}-r(k_1+k_2e^{-2ik})]\\&-\beta_2(1-re^{-ik})^2[k_1+k_2e^{ik}-r(k_1e^{2ik}+k_2)]\}/\{rD\},\end{aligned} \tag{75}$$

$$\begin{aligned}K_2 \equiv\ &\{\beta_1(r-1)^2[k_1+k_2e^{2ik}-r(k_1+k_2e^{-ik})]\\&-\beta_2(1-re^{-ik})^2[k_1+k_2e^{2ik}-r(k_1e^{2ik}+k_2e^{ik})]\}/\{D\},\end{aligned} \tag{76}$$

where

$$\begin{aligned}D =\ &[2m_1(\cos2\omega-1)+k_1+k_2][2m_2(\cos2\omega-1)+k_1+k_2]\\&-(k_1^2+k_2^2+2k_1k_2\cos2k).\end{aligned} \tag{77}$$

(2) Eq. (64):

$$c^0 \equiv \frac{-2k_2[\beta_2|1-re^{-ik}|^2+\beta_1|1-r|^2]}{(m_1+m_2)(k_1+k_2)(\omega_{,k})^2-k_1k_2},$$

$$c^1 \equiv \frac{2\beta_2(k_1+k_2)|1-re^{-ik}|^2}{(m_1+m_2)(k_1+k_2)(\omega_{,k})^2-k_1k_2}.$$

(3) Eq. (68):

$$B_1 = -\sin(\omega)\frac{(m_1+m_2)(k_1+k_2)+4m_1m_2(\cos\omega-1)}{2m_2(\cos\omega-1)+k_1+k_2},$$

$$B_2 = \frac{[(m_1+m_2)(k_1+k_2)+4m_1m_2(\cos\omega-1)]\cos(\omega)(\omega_{,k})^2-m_1m_2sin^2(\omega)(\omega_{,k})^2-k_1k_2\cos k}{k_1+k_2+2m_2(\cos\omega-1)},$$

$$\begin{aligned}
B_3 = {} & -2\beta_1^2(\bar{r}-1)\left\{(r-1)|r-1|^2\frac{2k_2(1-\cos k)+2(m_1+m_2)(\cos\omega-1)}{D}\right. \\
& \left. + \frac{2(r-1)}{k_1+k_2}|1-r|^2\right\} \\
& +2\beta_2^2(1-\bar{r}e^{ik})\left\{-(1-re^{-ik})|1-re^{-ik}|^2\frac{2k_1(1-\cos k)+2(m_1+m_2)(\cos\omega-1)}{D}\right. \\
& \left. + \frac{2(re^{-ik}-1)}{k_1+k_2}|1-re^{-ik}|^2\right\} \\
& +2\beta_1\beta_2(\bar{r}-1)\left\{(\bar{r}-1)(1-re^{-ik})^2\frac{-2e^{2ik}m_1(\cos\omega-1)-2m_2(\cos\omega-1)}{D}\right. \\
& \left. + \frac{2(r-1)}{k_1+k_2}|1-re^{-ik}|^2\right\} \\
& +2\beta_1\beta_2(1-\bar{r}e^{ik})\left\{(r-1)^2(1-\bar{r}e^{ik})\frac{-2e^{-2ik}m_1(\cos\omega-1)-2m_2(\cos\omega-1)}{D}\right. \\
& \left. + \frac{2(1-re^{-ik})}{k_1+k_2}|1-r|^2\right\},
\end{aligned}$$

$$B_4 = c^0B_6,$$

$$B_5 = c^1B_6,$$

$$B_6 = \frac{k_1\beta_2|1-re^{-ik}|^2+k_2\beta_1|1-r|^2}{k_1+k_2}.$$

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