Vector nonlinear Klein–Gordon lattices: General derivation of small amplitude envelope soliton solutions

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Abstract

Group velocity and group velocity dispersion for a wave packet in vectorial discrete Klein–Gordon models are obtained by an expansion, based on perturbation theory, of the linear system giving the dispersion relation and the normal modes. We show how to map this expansion on the multiple scale expansion in the real space and how to find nonlinear Schrödinger small amplitude solutions when a nonlinear on-site potential balances the group velocity dispersion effect. © 1999 Elsevier Science B.V.

1. Introduction

One of the most popular approaches used to determine the small amplitude envelope soliton solutions in nonlinear models is the well-known multiple scale expansion (MSE) technique [1]. This technique amounts to expanding the equations of motion on different time and space scales looking for wave-packet-like solutions; a wave packet is a superposition of plane waves whose frequencies and wave vectors lie in a narrow band, and it can be conveniently described by a plane wave with an amplitude that varies slowly in space and time. Increasing progressively the time and space scales one determines in a first step the carrier wave as a phonon mode of the linearized system, then deduces the partial differential equation that identifies the envelope phase velocity with the wave packet group velocity, and finally derives the NLS equation for the envelope whose diffusion coefficient is in fact the wave packet group velocity dispersion. An alternative method, commonly used in optics, consists in expanding the dispersion relations with respect to the carrier frequency and then in building at each order of this expansion an operator that acts on the envelope function [2]. MSE has been successfully applied to various nonlinear systems with scalar fields and the corresponding method adopted in optics has permitted the study of optical solitons in fibers. In this latter case one deals with electric field components which are not coupled at the linear order of the Maxwell equations. However, many nonlinear models of interest involve vectorial fields with coupled components at the linear order that give rise to dispersion relations with more than one branch: classical examples are given by multi-atomic lattices, or by lattices in which the mass at each site can move in a multidimensional space.

In this work, we show how to find small amplitude envelope soliton solutions in such vectorial lattice problems. The main difficulty with respect to the scalar case is to determine the relative amplitudes of the different components of the field. We will perform a perturbative expansion, around one wavenumber, of the linear system that gives the dispersion relations and the linear eigenmodes; then we will introduce an operator formalism analogous to that used in optics to obtain, from this expansion and from the nonlinear terms, the MSE equations, up to the NLS one.

An application of the method presented in this work can be found in a forthcoming paper [3], where the envelope soliton solutions of a helicoidal DNA model described by a radial and an angular degree of freedom for each site are derived.

2. Wave-packet in linear vectorial lattices

The NLS equation is obtained when a weak dispersion is balanced by a weak nonlinearity. In order to characterize the dispersion, let us first restrict our attention to the linear part of the system of interest. We start with a one-dimensional vectorial linear lattice model given by the equations of motion,

$$\frac{\partial^2 E(n, \alpha, t)}{\partial t^2} = - \sum_{n', \alpha'} J(n - n', \alpha, \alpha') E(n', \alpha', t), \tag{1}$$

where n, n' are the site indices, α, α' are the indices that label the components of the vectorial field $E(n, \alpha, t)$, and $J(n - n', \alpha, \alpha')$ are the force constants depending on $n - n'$ for translationally invariant systems.

Looking for plane wave solutions of the form

$$A V_l(q)\, e^{i(qn - \omega_l(q) t)} + \text{c.c.}, \tag{2}$$

where A is the wave amplitude, the equation of motion is mapped to the operator equation in the wave numbers space,

$$(\hat{J}(q) - \omega_l^2(q)) V_l(q) = 0, \tag{3}$$

where $\hat{J}(q)$ is the Fourier transform of the matrix $\hat{J}(n - n')$. The index l runs from 1 to the number of components of the vectorial field $E(n, \alpha, t)$; the eigenvalues functions $\omega_l^2(q)$ give the branches of the dispersion relation; the normal modes $V_l(q)$ are the orthonormalized eigenvectors of the matrix $\hat{J}(q) - \omega_l^2(q)$.

In order to investigate the dispersion, we now consider a wave-packet-like solution, i.e. a superposition of plane waves with wave numbers in a small interval,

$$E_l(n, t) = \int_{q_0 - \Delta q}^{q_0 + \Delta q} A(q)\, V_l(q)\, e^{i(qn - \omega_l(q) t)}\, dq + \text{c.c.} \tag{4}$$

For each q contributing to the wave packet the system of equations (3) must be fulfilled. The weakly dispersive case is obtained by considering only small deviations of q with respect to the wavevector q_0 corresponding to the center of the wavepacket. To measure this deviation, the wavevector q is written $q = q_0 + \epsilon q_1$, where $\epsilon \ll 1$.

Eq. (3) is solved, $\forall q_1$ in the integration range, by a perturbative technique.

The operator $\hat{J}(q_0 + \epsilon q_1)$ can be expanded in Taylor series as $\hat{J}(q_0) + \epsilon \hat{J}'(q_0)\, q_1 + \epsilon^2 \hat{J}''(q_0)\, q_1^2/2 + \dots$ The quantities $\epsilon \hat{J}'(q_0)\, q_1$, $\epsilon^2 \hat{J}''(q_0)\, q_1^2/2$ are small perturbations with respect to the unperturbed operator $\hat{J}(q_0)$, whose eigenvalues are $\omega_l^2 = \omega_l^2(q_0)$ and whose eigenvectors $V_l = V_l(q_0)$ constitute a complete basis.

According to standard perturbation theory [4] we write the expansions of the eigenvectors and eigenvalues,

$$V_l(q_0 + \epsilon q_1) = V_l + \epsilon V_l^{(1)} q_1 + \epsilon^2 V_l^{(2)} q_1^2/2 + \dots, \tag{5}$$

$$\omega_l(q_0 + \epsilon q_1) = \omega_l + \epsilon \omega_l^{(1)} q_1 + \epsilon^2 \omega_l^{(2)} q_1^2/2 + \dots \tag{6}$$

Eq. (3) has to be solved at each expansion order,

at order ϵ^0: $\quad \hat{J} V_l = \omega_l^2 V_l,$ \hfill (7)

at order ϵ^1: $\quad (\hat{J} V_l^{(1)} + \hat{J}' V_l) q_1 = (2\omega_l \omega_l^{(1)} V_l + \omega_l^2 V_l^{(1)}) q_1,$ \hfill (8)

at order ϵ^2: $\quad (\hat{J}' V_l^{(1)} + \frac{1}{2}\hat{J}'' V_l + \frac{1}{2}\hat{J} V_l^{(2)}) q_1^2 = (\omega^{(1)}{}_l^2 V_l + \omega_l \omega_l^{(2)} V_l + 2\omega_l \omega_l^{(1)} V_l^{(1)} + \frac{1}{2}\omega_l^2 V_l^{(2)}) q_1^2.$ \hfill (9)

At order ϵ^0, one solves the unperturbed problem determining V_l and ω_l. At order ϵ, one determines $V_l^{(1)}$, $\omega_l^{(1)}$: imposing $V_l^{(1)}$ to be orthogonal to V_l to guarantee the normalization of $V_l(q_0 + \epsilon q_1)$, the scalar product of (8) with V_m^* $(m \neq l)$ gives

$$V_l^{(1)} = \sum_{m \neq l} \alpha_m V_m, \tag{10}$$

$$\alpha_m = \frac{V_m^* \hat{J}' V_l}{\omega_l^2 - \omega_m^2}, \quad m \neq l, \tag{11}$$

and that with V_l^* gives

$$\omega_l^{(1)} = \frac{V_l^* \hat{J}' V_l}{2\omega_l}. \tag{12}$$

At order ϵ^2, one determines $\omega_l^{(2)}$ by multiplying (9) by V_l^*,

$$\omega_l^{(2)} = \frac{1}{\omega_l} \left(V_l^* \frac{\hat{J}''}{2} V_l - \omega^{(1)}{}_l^2 + \sum_{m \neq l} \frac{|V_m^* \hat{J}' V_l|^2}{\omega_l^2 - \omega_m^2} \right). \tag{13}$$

We assume, for the sake of simplicity, that the eigenmodes of J (see (3)) are not degenerate, but the generalization of the degenerate case is possible with the standard perturbation theory.

The phase of each component of (4) can be expanded around the central wave number q_0, up to second order in $\epsilon q_1 = q - q_0$ using the values of $\omega_l^{(1)}$ and $\omega_l^{(2)}$ determined above,

$$E_l(n, t) = e^{i(q_0 n - \omega_l(q_0) t)} \epsilon \int_{-\Delta q/\epsilon}^{+\Delta q/\epsilon} A(q_0 + \epsilon q_1) V_l(q_0 + \epsilon q_1)$$

$$\times \exp\{i \epsilon q_1 (n - \omega_l^{(1)}(q_0) t) - \frac{1}{2} i \epsilon^2 q_1^2 \omega_l^{(2)}(q_0) t\} \, dq_1 + \text{c.c.} \tag{14}$$

Under this form, $E_l(n, t)$ appears as a plane wave, henceforth called the carrier wave, with an amplitude that depends on space and time and which corresponds to the integral of Eq. (14), $E_l(n, t) = F(n, t) \exp[i(q_0 n - \omega_l(q_0) t)] + \text{c.c.}$ The fact that $\omega_l^{(1)}(q_0)$, $\omega_l^{(2)}(q_0)$ obey relations (12) and (13) ensures that this wave packet is a solution of the original Eq. (1), up to the order of the various expansions.

In order to extend the study to the nonlinear case it is useful to express these conditions under the form of an equation in the space–time coordinates for the amplitude. Let us introduce the quantity

$$A(n,t) = \int\limits_{-\Delta q/\epsilon}^{+\Delta q/\epsilon} A(q_0 + \epsilon q_1) \exp\{i\epsilon q_1(n - \omega_l^{(1)}(q_0) t) - \tfrac{1}{2}i\epsilon^2 q_1^2 \omega_l^{(2)}(q_0) t\}\, dq_1. \tag{15}$$

Eq. (15) shows that $A(n,t)$ slowly varies in space and time. In the spirit of the multiple scale expansion, it is natural to introduce the slow variables $x_1 = \epsilon n$, $t_1 = \epsilon t$ and $t_2 = \epsilon^2 t$ so that $A(n,t)$ can be written as

$$A(n,t) = A(x_1, t_1, t_2) = \int\limits_{-\Delta q/\epsilon}^{+\Delta q/\epsilon} A(q_0 + \epsilon q_1) \exp\{iq_1(x_1 - \omega_l^{(1)}(q_0) t_1) - \tfrac{1}{2}iq_1^2 \omega_l^{(2)}(q_0) t_2\}\, dq_1, \tag{16}$$

or

$$A(x_1, t_1, t_2) = A(s_1, t_2) = \int\limits_{-\Delta q/\epsilon}^{+\Delta q/\epsilon} A(q_0 + \epsilon q_1) \exp\{iq_1 s_1 - \tfrac{1}{2}iq_1^2 \omega_l^{(2)}(q_0) t_2\}\, dq_1, \tag{17}$$

with the introduction of the variable $s_1 = x_1 - \omega_l^{(1)}(q_0) t_1$ to switch to the frame moving at the group velocity of the carrier wave.

Using the relation $(\partial A/\partial x_1) = (\partial A/\partial s_1) = i\langle q_1 \rangle \equiv \int_{-\Delta q/\epsilon}^{+\Delta q/\epsilon} iq_1 A(q_0 + \epsilon q_1) \exp\{iq_1 s_1 - \tfrac{1}{2}iq_1^2 \omega_l^{(2)}(q_0) t_2\}\, dq_1$ that derives directly from Eqs. (16) and (17), and the expansion (5) of $V(q_0 + \epsilon q_1)$, the amplitude F of the wave can be expressed as a function of $A(s_1, t_2)$ by the relation

$$F(x_1, t_1, t_2) = \epsilon\left(V_l - i\epsilon V_l' \frac{\partial}{\partial x_1}\right) A(x_1, t_1, t_2). \tag{18}$$

From (16) and (17), we directly derive the equations of motions of A as a function of the slow space–time variables,

$$\left(\frac{\partial A}{\partial t_1} + \omega_l^{(1)} \frac{\partial A}{\partial x_1}\right) = 0, \tag{19}$$

and

$$i\frac{\partial A}{\partial t_2} + \frac{\omega_l^{(2)}}{2} \frac{\partial^2 A}{\partial s_1^2} = 0, \tag{20}$$

where $\omega_l^{(1)}$ and $\omega_l^{(2)}$ are then the group velocity and the group velocity dispersion of the wave packet and determine the velocity and the spread out of the envelope function. Eq. (18) shows that V_l' determines the first order correction to the direction of the vectorial field solution.

3. Nonlinear vectorial lattice

We now consider the full equation of motion, including nonlinear on-site potential terms. Extra nonlinear terms depending on time derivatives may also appear in the case of non-Cartesian coordinates systems,

$$\frac{\partial^2 E(n,\alpha,t)}{\partial t^2} = -\sum_{n',\alpha'} J(n-n',\alpha,\alpha')\, E(n',\alpha',t)$$

$$+ \sum_{d=0}^{2}\sum_{k=0}^{d}\sum_{\alpha'',\alpha'\leqslant\alpha''} c_{d,k}^{\alpha}(\alpha',\alpha'')\, E^{(k)}(n,\alpha',t)\, E^{(d-k)}(n,\alpha'',t)$$

$$+ \sum_{d=0}^{2}\sum_{k=0}^{d}\sum_{j=0}^{k}\sum_{\alpha''',\alpha''\leqslant\alpha''',\alpha'\leqslant\alpha''} C_{d,k,j}^{\alpha}(\alpha',\alpha'',\alpha''')\, E^{(j)}(n,\alpha',t)\, E^{(k-j)}(n,\alpha'',t)\, E^{(d-k)}(n,\alpha''',t),$$

$$(21)$$

where $E^{(j)}(n,\alpha,t)$ indicates the jth time derivative of $E(n,\alpha,t)$, and $c_{d,k}^{\alpha}(\alpha',\alpha'')$, $C_{d,k,j}^{\alpha}(\alpha',\alpha'',\alpha''')$ are the quadratic and cubic nonlinear terms numerical coefficients. Index d is the total time derivative order of each term. The terms with $d=0$ are the nonlinear potential force terms; the others derive from the kinetic energy in the case of non-Cartesian coordinates so that $d \leqslant 2$.

The quadratic terms in (21) give rise to second harmonic and constant terms that have to be included as additional smaller corrections if we look for a small amplitude solution,

$$E_l(n,t) = \epsilon e^{i(q_0 n_0 - \omega_l t_0)}\left(V_l - i\epsilon V_l^{(1)}\frac{\partial}{\partial x_1}\right)A(x_1,t_1,t_2) + \epsilon^2 e^{2i(q_0 n_0 - \omega_l t_0)}\gamma_l A^2(x_1,t_1,t_2)$$

$$+ \epsilon^2 \mu_l |A(x_1,t_1,t_2)|^2 + O(\epsilon^3).$$

$$(22)$$

We are interested in situations where dispersion can balance nonlinearity, and therefore they have to be measured by the same scaling parameter ϵ. While the overall ϵ factor was not important in the linear case, it must be explicitly included in the nonlinear case.

We solve the equation of motion (21) on the three characteristic magnitude scales of the wave packet. At order ϵ we get ω_l, V_l from Eq. (7).

At order ϵ^2 we get for the wave packet term expressed in the form (4) the system of equations (8) for each q_1 in the integration range. After integration on the envelope distribution this gives rise to the equation in the anti-transformed Fourier space

$$\left(2\omega_l V_l\frac{\partial}{\partial t_1} + (\hat{J} - \omega_l^2)V_l^{(1)}\frac{\partial}{\partial x_1} + \hat{J}'V_l\frac{\partial}{\partial x_1}\right)A(x_1,t_1,t_2) = 0.$$

$$(23)$$

In fact from (16), the average wave numbers deviation is $\langle q_1\rangle = -i\partial A/\partial x_1$ and the averaged frequency deviation is in the same way $\langle\Delta\omega_l\rangle = \langle\omega_l^{(1)}q_1\rangle = i\partial A/\partial t_1$.

By scalar product of (23) and $V_m^* \,\forall m \neq l$ we obtain the components α_m (11) of $V_l^{(1)}$ (10) on the base $\{V_m\}$ and by scalar product of (23) and V_l^* we obtain Eq. (19) with $\omega_l^{(1)}$ defined by (12).

At the same order of expansion one determines the vectors γ_l, μ_l collecting the terms of corresponding order (ϵ^2) and phase in the equation of motion (21) in which the solution form (22) has been inserted [1]. One then obtains γ_l by solving the algebraic system

$$(\hat{J}(2q_0) - 4\omega_l^2(q_0))\gamma_l = \sum_{d=0}^{2}\sum_{k=0}^{d}\sum_{\alpha'',\alpha'\leqslant\alpha''} c_{d,k}(\alpha',\alpha'')\,(-i\omega_l)^d\, V_l(\alpha')\, V_l(\alpha''),$$

$$(24)$$

where $c_{d,k}(\alpha',\alpha'')$ is the vector of components $c_{d,k}^{\alpha}(\alpha',\alpha'')$, each derivative with respect to t_0 giving a factor $(-i\omega_l)$. And μ_l is obtained from the system

[1] Note that if $J(0)$ has some null columns the linear system solution is defined except for some constant components. They have to be added as order ϵ terms in (22), enter in the r.h.s. of (25), and are then solved with the $O(\epsilon^2)$ equations [3]; the final $O(\epsilon)$ result is in this case a combination of oscillating envelope soliton and nonoscillating soliton contributions.

$$\hat{J}(0)\,\pmb{\mu}_l = \sum_{d=0}^{2}\sum_{k=0}^{d}\sum_{\alpha'',\alpha'\leqslant\alpha''} c_{d,k}(\alpha',\alpha'')\,[\,(i\omega_l)^k(-i\omega_l)^{d-k}V_l^*(\alpha')\,V_l(\alpha'')$$
$$+ (-i\omega_l)^k(i\omega_l)^{d-k}V_l^*(\alpha'')\,V_l(\alpha')\,]. \tag{25}$$

At order ϵ^3, from (21) and (22) for the terms in $e^{i(q_0n_0-\omega_l(q_0)\,t_0)}$, one obtains the system of equations

$$\left([\,(\tfrac{1}{2}\hat{J}''-\omega_l^{(1)\,2})V_l + (\hat{J}'-2\omega_l\omega_l^{(1)})V_l^{(1)} + (\tfrac{1}{2}(\hat{J}-\omega_l^2)V^{(2)})]\frac{\partial^2}{\partial s_1^2} + 2i\omega_l V_l\frac{\partial}{\partial t_2}\right)A(s_1,t_2)$$
$$+ \pmb{Q}|A(s_1,t_2)|^2 A(s_1,t_2) = 0, \tag{26}$$

where

$$\pmb{Q} = \sum_{d=0}^{2}\sum_{k=0}^{d}\sum_{\alpha'',\alpha'\leqslant\alpha''} c_{d,k}(\alpha',\alpha'')\,[\,(i\omega_l)^k(-2i\omega_l)^{d-k}V_l^*(\alpha')\,\gamma_l(\alpha'')$$

$$+ (-2i\omega_l)^k(i\omega_l)^{d-k}V_l^*(\alpha'')\,\gamma_l(\alpha')\,] + 2\sum_{d=0}^{2}\sum_{\alpha'',\alpha'\leqslant\alpha''} c_{d,0}(\alpha',\alpha'')(-i\omega_l)^d\mu_l(\alpha')\,V_l(\alpha'')$$

$$+ \sum_{d=0}^{2}\sum_{k=0}^{d}\sum_{j=0}^{k}\sum_{\alpha''',\alpha''\leqslant\alpha''',\alpha'\leqslant\alpha''} C_{d,k,j}(\alpha',\alpha'',\alpha''')\,[\,(-i\omega_l)^j(-i\omega_l)^{k-j}(i\omega_l)^{d-k}V_l(\alpha')\,V_l(\alpha'')\,V_l^*(\alpha''')$$
$$+ (-i\omega_l)^j(i\omega_l)^{k-j}(-i\omega_l)^{d-k}V_l(\alpha')\,V_l^*(\alpha'')\,V_l(\alpha''')$$
$$+ (i\omega_l)^j(-i\omega_l)^{k-j}(-i\omega_l)^{d-k}V_l^*(\alpha')\,V_l(\alpha'')\,V_l(\alpha''')\,]. \tag{27}$$

The first term of Eq. (26) corresponds to the third order expansion (9) of the linear operator equation (3) applied to the wave packet (terms in $e^{i(q_0n_0-\omega_l(q_0)\,t_0)}$ in (22)), in the moving reference frame used in (20), $\langle q_1\rangle = -i(\partial/\partial s_1)A(s_1,t_2)$, and $\langle\omega_l^{(2)}q_1^2/2\rangle = \langle\Delta(\Delta(\omega_l))\rangle = i(\partial/\partial t_2)A(s_1,t_2)$.

The first two terms on the right-hand side of the nonlinear coefficients vector $\pmb{Q}$ arise from the double product, in the nonlinear quadratic force terms in (21), between $O(\epsilon)$ and $O(\epsilon^2)$ components of (22); the last two terms come from the nonlinear cubic force terms in (21) when considering just the $O(\epsilon)$ terms in $E_l(n,t)$.

Multiplying Eq. (26) by V_l^* we obtain the NLS equation

$$\left(P\frac{\partial^2}{\partial s_1^2} + i\frac{\partial}{\partial t_2}\right)A(s_1,t_2) + Q|A(s_1,t_2)|^2 A(s_1,t_2) = 0, \tag{28}$$

where

$$P = \frac{1}{2\omega_l}\left(V_l^*\frac{\hat{J}''}{2}V_l - \left(\frac{V_l^*\hat{J}'V_l}{2\omega_l}\right)^2 + \sum_{m\neq l}\frac{|V_m^*\hat{J}'V_l|^2}{\omega_l^2-\omega_m^2}\right), \tag{29}$$

and

$$Q = \frac{V_l^*\pmb{Q}}{2\omega_l}. \tag{30}$$

The first part of Eq. (28) is Eq. (20) for the wave packet with $2P = \omega_l^{(2)}$ given by (13) to which is now added the nonlinear part with coefficient Q. If $PQ > 0$ then the effect of the amplitude-dependent nonlinear potential well in (28) balances the wave packet group velocity dispersion giving rise to the stable envelope soliton solution [1].

4. Summary

The main outlines of the approach presented in this paper are the following. The envelope-soliton-like solutions arise in systems with weak dispersion and weak nonlinearity by two parallel series expansions driven by a common expansion parameter (ϵ): on one hand the weakness of the diffusion, for a wave-packet-like solution, allows an expansion of the equations that regulate the space–time behaviour of the solution on different scales; on the other hand the weak nonlinearity, for small amplitude solutions, allows to write the equations of motion at increasing orders of accuracy introducing the nonlinear terms in a progressive way. For scalar fields the Taylor series expansion of dispersion relations gives directly the diffusive part for the envelope equations of motion. Vectorial fields are instead characterized by a linear part which gives rise, in the q space, to an eigenvalue (dispersion relations) and eigenvector (relative amplitude of the different components) problem (3); to obtain the correct expansion in multiple scales it is then necessary to apply the perturbation theory (5), (6). Finally, to combine this perturbative expansion with the nonlinear one, we antitransform Eqs. (8), (9) as done in (23), (26).

Following the approach introduced in this paper it is straightforward to derive the NLS equation for every nonlinear vectorial lattice with on-site nonlinearities and with an arbitrary number of components. For more complex systems this could even be programmed in symbolic languages to provide a fully automatic method. After having identified the nonlinear coefficients $c_{d,k}^{\alpha}(\alpha', \alpha'')$ and $C_{d,k,j}^{\alpha}(\alpha', \alpha'', \alpha''')$ in the equation of motion (21), there are only algebraic systems to solve: one has to solve the eigenvectors $V_l(q_0)$ and the eigenvalues $\omega_l(q_0)$ of the matrix $\hat{J}(q_0)$, then the systems (24) and (25) for γ_l and μ_l, and to derive P from (29) and Q from (27) and (30). From (28) one then obtains, if $PQ \geqslant 0$, the envelope function $A(x_1, t_1, t_2)$ that, inserted into (22) together with the eigenvector correction (10), (11), gives the complete $O(\epsilon^2)$ solution we are looking for.

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