

Nonlinear model of intramolecular excitations on a multileg ladder lattice

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The exactly integrable model of nonlinear intramolecular excitations on a multileg ladder lattice is proposed. Since it is rather general, the model permits a number of physically interesting ramifications related to the striplike and the bunchlike biological and condensed matter systems as well as to the arrays of linearly and nonlinearly coupled optical fibers. The principal possibility to model an external magnetic field parallel to the ladder legs within the framework of inverse scattering transform is pointed out. The one-soliton solutions of two-leg and three-leg ladder models are found and analyzed. Apart from the spatially constricted translational mode typical to the traditional one-chain soliton, the interchain beating mode as well as the circular traveling modes redistributing the excitations between the chains are revealed in complete accordance with linear limits. [S1063-651X(99)51309-3]

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The models of a nonlinear Schrödinger type have played an exceptional role in physical applications already for more than three decades. They arise in rather different physical systems where the balance between dispersion and nonlinearity produces the fundamental entity known as a soliton. The scope of such models stretches from the transport phenomena in low-dimensional biological [1–3] and condensed matter [3–6] systems to two-dimensional self-focussing [7,8] and one-dimensional self-modulation [7] of light in nonlinear media to say nothing of light pulse propagation in optical fibers [9,10] and electric pulse propagation in nonlinear transmission lines [11]. The most intriguing ones are the multicomponent nonlinear models supporting linear [12,13] or nonlinear [8,9,14] couplings between their components thereby prompting rather sophisticated effects of mode-mode interactions. However, as a rule only some of them are integrable and in particular those admitting equal contributions from cross-phase and self-phase modulation effects [8]. Here, apart from the well-known Manakov model [8], which has served as an integrable model for the so-called incoherent solitons, it is worthwhile to mention that its discretized multicomponent versions just recently appeared in the literature [15,16]. Though being rare ones the integrable models when chosen appropriately are often used to be good zero approximations as applied to real physical systems [17–20]. At last in the papers [21–24] a number of fairly general two-component models closely related to different physical situations have been considered. Among them we would like to stress those dealing with the linear and nonlinear intercomponent couplings combined [21–23] as the most direct continuous prototypes of discrete multicomponent nonlinear integrable model has to be presented in this Rapid Communication.

Thus, the main reason of our activity is to develop a discrete nonlinear integrable model pretending to be a zero approximation at least for such known physically motivated models as arrays of tunnel-coupled nonlinear optical fibers [25–27] or models for transport of excitation energy and

charge in transversely coupled biological macromolecules [1–3]. Forestalling, in some respect the model has even surpassed our expectations though its nonlinear terms turned out to be somewhat artificial, as it usually occurred with other discrete integrable nonlinear models [15,16,28]. We will discuss all these aspects in context of each particular property of the model of interest.

For the sake of definiteness we will follow here the terminology of nonlinear transport phenomena and prescribe the quantities $q_\alpha(n)$ and $r_\alpha(n)$ to be the excitation amplitudes of molecule sited on α th chain and n th unit cell. The longitudinal numerical coordinate n is supposed to run from minus to plus infinity, whereas the transverse one α from unity to the number of chains (legs) M . The exactly integrable evolution model dealing with the nonlinear intramolecular excitations on M -leg ladder lattice reads as follows:

$$\begin{aligned}
 i\dot{q}_\alpha(n) + \sum_{\beta=1}^M t_{\alpha\beta} q_\beta(n) + [q_\alpha(n+1) + q_\alpha(n-1)] \\
 \times \left[1 + \sum_{\beta=1}^M q_\beta(n) r_\beta(n) \right] \\
 = \sum_{\beta=1}^M [q_\alpha(n-1) q_\beta(n) - q_\alpha(n) q_\beta(n-1)] r_\beta(n) \quad (1) \\
 - i\dot{r}_\alpha(n) + \sum_{\beta=1}^M r_\beta(n) t_{\beta\alpha} + [r_\alpha(n+1) + r_\alpha(n-1)] \\
 \times \left[1 + \sum_{\beta=1}^M r_\beta(n) q_\beta(n) \right] \\
 = \sum_{\beta=1}^M [r_\alpha(n+1) r_\beta(n) - r_\alpha(n) r_\beta(n+1)] q_\beta(n), \quad (2)
 \end{aligned}$$

where $\alpha=1,2,3,\dots,M$ and the interchain linear coupling constants $t_{\alpha\beta}$ are supposed to be arbitrary for the time being. Here the dot stands for the derivative with respect to dimensionless time τ .

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Being rather general the model (1) and (2) permits a number of physically interesting ramifications obtainable by merely imposing appropriate restrictions on the coupling constants $t_{\alpha\beta}$. Thus, we are able to model the nonlinear excitations on a multileg ladder lattice unrolled into the two-dimensional strip or combined into the three-dimensional bunch of tightly bound chains. Moreover, we are in a position to apply an external magnetic field parallel to the ladder legs in a way similar to that described by Feynman [29].

Inspecting the kind of nonlinearity the model (1) and (2) possesses we see that it has the thorough physically motivated justification only in continuous limit when the role of longitudinal localized modes is negligible. Thus, at $M=2$ and the absence of interchain linear couplings $t_{\alpha\beta} \equiv 0$ ($\alpha \neq \beta$) we can readily recognize in continuous version of Eqs. (1) and (2) the famous Manakov model [8]. Nevertheless, even at intermediate spatial localization when the nonlinear

wave packet occupies two or three unit cells the difference between the physical and modeled nonlinearities can be reasonably taken into account by the perturbation technique similar to that developed in our previous works [17,18]. For example, the parameters of Peierls-Nabarro potential relief obtained by means of perturbation theory [17,18] for the nonlinear Davydov-Kislukha model [4] turned out to be in good keeping with those calculated numerically [30]. Moreover, even the so-called intrinsic localized modes [31,32,18] have actually been described at first within the framework of the perturbation theory [17]. Of course, the effects of strong localization should be treated within the framework of other approaches, e.g. that worked out by the Spatschek's team [33,34].

Before proceeding with some particular cases of our model (1) and (2) we will prove its integrability. Indeed introducing two auxiliary linear operators $L(n|z)$ and $A(n|z)$ as

$$L(n|z) = \begin{pmatrix} zI & F(n)E \\ EG(n) & z^{-1}I \end{pmatrix}, \quad (3)$$

$$A(n|z) = \begin{pmatrix} iz^2I - iF(n)EEG(n-1) + iT & izF(n)E - iz^{-1}F(n-1)E \\ izEG(n-1) - iz^{-1}EG(n) & -iz^{-2}I + iEG(n)F(n-1)E \end{pmatrix}, \quad (4)$$

we see that the model (1) and (2) follows from the zero-curvature condition

$$\dot{L}(n|z) = A(n+1|z)L(n|z) - L(n|z)A(n|z), \quad (5)$$

thereby confirming its integrability. Here the quantities I , E , T , and $F(n)$, $G(n)$ stand for $M \times M$ submatrices defined by

$$I \equiv [I_{\alpha\beta}] = [\delta_{\alpha\beta}], \quad (6)$$

$$E \equiv [E_{\alpha\beta}] = [1], \quad (7)$$

$$T \equiv [t_{\alpha\beta}], \quad (8)$$

$$F(n) \equiv [F_{\alpha\beta}(n)] = [iq_{\alpha}(n)\delta_{\alpha\beta}]/\sqrt{M}, \quad (9)$$

$$G(n) \equiv [G_{\alpha\beta}(n)] = [i\delta_{\alpha\beta}r_{\beta}(n)]/\sqrt{M}. \quad (10)$$

A comprehensive analysis handled by the inverse scattering transform shows that one-soliton amplitudes cancel the left-hand terms in Eqs. (1) and (2) identically and convert the initial multileg model (1) and (2) into the more simple one,

$$i\dot{q}_{\alpha}(n) + \sum_{\beta=1}^M t_{\alpha\beta}q_{\beta}(n) + [q_{\alpha}(n+1) + q_{\alpha}(n-1)] \times \left[1 + \sum_{\beta=1}^M q_{\beta}(n)r_{\beta}(n) \right] = 0, \quad (11)$$

$$-i\dot{r}_{\alpha}(n) + \sum_{\beta=1}^M r_{\beta}(n)t_{\beta\alpha} + [r_{\alpha}(n+1) + r_{\alpha}(n-1)] \times \left[1 + \sum_{\beta=1}^M r_{\beta}(n)q_{\beta}(n) \right] = 0, \quad (12)$$

$$\alpha = 1, 2, 3, \dots, M.$$

Provided the matrix $[t_{\alpha\beta}]$ is Hermitian $t_{\beta\alpha} \equiv t_{\alpha\beta}^*$ this last model (11) and (12) gains a direct physical implication inasmuch as then its amplitudes could be linked by one of the reductions $r_{\alpha}(n) = q_{\alpha}^*(n)$ or $r_{\alpha}(n) = -q_{\alpha}^*(n)$. Indeed as far as the initial Eqs. (1) and (2) and simplified Eqs. (11) and (12) conserve the quantity $\sum_{m=-\infty}^{\infty} \ln[1 + \sum_{\beta=1}^M q_{\beta}(n)r_{\beta}(n)]$ we can introduce the corrected amplitudes

$$Q_{\alpha}(n) = q_{\alpha}(n) \sqrt{\frac{\ln \left[1 + \sum_{\beta=1}^M q_{\beta}(n)r_{\beta}(n) \right]}{\sum_{\beta=1}^M q_{\beta}(n)r_{\beta}(n)}}, \quad (13)$$

$$R_\alpha(n) = r_\alpha(n) \sqrt{\frac{\ln \left[1 + \sum_{\beta=1}^M q_\beta(n) r_\beta(n) \right]}{\sum_{\beta=1}^M q_\beta(n) r_\beta(n)}}, \quad (14)$$

manifesting at $r_\alpha(n) = q_\alpha^*(n)$ all necessary features of probability amplitudes. Of course, both models can be easily reformulated in terms of $Q_\alpha(n)$ and $R_\alpha(n)$ should the need arise.

In what follows we analyze the amplitudes of the one-soliton solution under the restrictions $t_{\beta\alpha} = t_{\alpha\beta}^*$ and $r_\alpha(n) = q_\alpha^*(n)$ (the reduced amplitudes),

$$q_\alpha(n) = \frac{a_\alpha(\tau) \operatorname{sh} \mu \exp[ipn - 2i\tau \operatorname{ch} \mu \cos p]}{\sqrt{\sum_{\beta=1}^M a_\beta(\tau) a_\beta^*(\tau) \operatorname{ch}[\mu(n-x) - 2\tau \operatorname{sh} \mu \sin p]}} \quad (15)$$

$$r_\alpha(n) = q_\alpha^*(n), \quad (16)$$

$$\alpha = 1, 2, 3, \dots, M.$$

Here μ , p , x , and $a_\alpha(\tau)$ are the constant real and time dependent complex integration parameters respectively determined through the scattering data of auxiliary spectral problem by some one-to-one relations. In particular the quantities $a_\alpha(\tau)$ should satisfy to the following set of ordinary differential equations:

$$\dot{a}_\alpha(\tau) = i \sum_{\beta=1}^M t_{\alpha\beta} a_\beta(\tau), \quad \alpha = 1, 2, 3, \dots, M. \quad (17)$$

Being the one-soliton ones the amplitudes (15) and (16) are applicable to each of models (1), (2), and (11), (12) on an equal footing.

Let us clarify the meaning of integration parameters. Thus, the coordinate x turns out to be the mean longitudinal coordinate of soliton distribution due to the fact that the identity

$$\frac{\sum_{\alpha=1}^M \sum_{n=-\infty}^{\infty} n Q_\alpha(n) R_\alpha(n)}{\sum_{\alpha=1}^M \sum_{n=-\infty}^{\infty} Q_\alpha(n) R_\alpha(n)} \equiv x \quad (18)$$

when calculated on the one-soliton amplitudes (15) and (16) is fulfilled. Further, the quantity $2(\operatorname{sh} \mu \sin p)/\mu$ gives the soliton longitudinal velocity while the quantity $1/\mu$ determines the typical longitudinal size of soliton distribution. At last the amplitudes $a_\alpha(\tau)$ ($\alpha = 1, 2, 3, \dots, M$) describe the temporal transverse redistribution of soliton density. Indeed, the fraction of one-soliton density located on the α th chain in accordance with Eqs. (15), (16), and (13), (14) is found to be

$$\frac{Q_\alpha(n) R_\alpha(n)}{\sum_{\beta=1}^M Q_\beta(n) R_\beta(n)} = \frac{a_\alpha(\tau) a_\alpha^*(\tau)}{\sum_{\beta=1}^M a_\beta(\tau) a_\beta^*(\tau)} \equiv \frac{a_\alpha(\tau) a_\alpha^*(\tau)}{\sum_{\beta=1}^M a_\beta(0) a_\beta^*(0)}, \quad (19)$$

where the last step has been assisted by the evolution equations (17) and Hermiticity of interchain coupling matrix $[t_{\alpha\beta}]$ combined. We will demonstrate the actual temporal interchain redistribution of excitations for the particular cases admitting the physical applications.

Thus, putting $M=2$ and $t_{\alpha\beta} = (1 - \delta_{\alpha\beta})t$ with t to be real we obtain from Eqs. (1) and (2) the model of nonlinear intermolecular excitations on two-leg ladder lattice closely related to that on double helix DNA macromolecule. Then solving Eq. (17) yields

$$a_\alpha(\tau) = \frac{1}{2} \sum_{\beta=1}^2 [e^{i\tau} + (-1)^{\alpha-\beta} e^{-i\tau}] a_\beta(0), \quad \alpha = 1, 2 \quad (20)$$

and consequently

$$\frac{a_\alpha(\tau) a_\alpha^*(\tau)}{\sqrt{\sum_{\beta=1}^3 a_\beta(0) a_\beta^*(0)}} = \frac{1}{2} - \frac{(-1)^\alpha}{2} [\cos 2\phi \cos(2t\tau) + \sin(\delta_1 - \delta_2) \sin 2\phi \sin(2t\tau)], \quad \alpha = 1, 2, \quad (21)$$

where the parametrization $a_1(0) = \exp(i\delta_1) \cos \phi$, $a_2(0) = \exp(i\delta_2) \sin \phi$ has been adopted. From Eq. (21) it is clearly seen the presence of interchain beating mode redistributing the excitations between the chains. The beating amplitude is equal to $\sqrt{\cos^2 2\phi + \sin^2(\delta_1 - \delta_2) \sin^2 2\phi}$ and can be regulated from zero to unity by means of parameters δ_1 , δ_2 , and ϕ of initial transverse distribution. Conversely, the beating frequency t/π has the fundamental physical origin and is determined exclusively by the interchain linear coupling constant t regardless to any particular solution. Moreover, the effect of interchain beating could be observable only in systems with interchain linear couplings and is principally impossible, e.g., in those of Manakov type [8,15,16].

Now let us consider the case when $M=3$ and $t_{\alpha\beta} = t \exp(-i\Phi/3) \Delta(\alpha - \beta + 1) + t \exp(i\Phi/3) \Delta(\alpha - \beta - 1)$. Here $\Delta(\gamma)$ stands for unity if the number γ is equal to zero or is divisible by three and for zero otherwise. Then at $\Phi = 0$ the model (1) and (2) describe the chargeless nonlinear intramolecular excitations (or charged ones without external magnetic field) on a three-leg ladder lattice. This model is closely related to the model established for amid-I excitations on a α -helix protein macromolecule [1-3]. When the quantity Φ is nonzero it is worthwhile to identify it with the dimensionless magnetic flux through the triangular area element with vortices situated on molecules of the same unit cell,

$$\Phi = \frac{e}{c\hbar} |\mathbf{B}| S, \quad (22)$$

bearing in mind the most general integrable model of charged excitations on a three-leg lattice structure. Here S is the area of triangular element just referred to. The magnetic field \mathbf{B} is supposed to be directed along the positive direction of discrete longitudinal coordinate n . Solving the evolution equations (17) gives rise to

$$a_{\alpha}(\tau) = \frac{1}{3} \exp[2it\tau \cos(\Phi/3)] \sum_{\beta=1}^3 a_{\beta}(0) + \frac{1}{3} \exp[2it\tau(\Phi/3 - 2\pi/3)] \sum_{\beta=1}^3 a_{\beta}(0) e^{2\pi i(\alpha-\beta)/3} + \frac{1}{3} \exp[2it\tau(\Phi/3 + 2\pi/3)] \sum_{\beta=1}^3 a_{\beta}(0) e^{-2\pi i(\alpha-\beta)/3}, \quad \alpha = 1, 2, 3. \quad (23)$$

In general the corresponding expression for the one-soliton density located on the α th chain (19) looks rather cumbersome. So we prefer to write down a particular one,

$$\frac{a_{\alpha}(\tau) a_{\alpha}^*(\tau)}{\sqrt{\sum_{\beta=1}^3 a_{\beta}(0) a_{\beta}^*(0)}} = \frac{1}{3} + \frac{2}{9} \cos[2\sqrt{3}t\tau \sin(\Phi/3) - 2\pi\alpha/3] + \frac{2}{9} \cos[2\sqrt{3}t\tau \sin(\pi/3 - \Phi/3) - 2\pi\alpha/3] + \frac{2}{9} \cos[2\sqrt{3}t\tau \sin(\pi/3 + \Phi/3) + 2\pi\alpha/3], \quad \alpha = 1, 2, 3, \quad (24)$$

when the whole initial soliton density is concentrated on the third chain $a_{\alpha}(0) = \delta_{\alpha 3} \exp(i\delta_3)$. According to this formula the transverse redistribution of soliton density is carried out by three circular traveling waves with frequencies regulated by an external magnetic field. In general all three modes are different and even incommensurate ones though at certain particular values of the magnetic field the effects of two-mode degeneration or two-mode degeneration accompanied by vanishing of the third mode are possible to observe.

In summary, we have developed the exactly integrable nonlinear model on multileg ladder lattice strongly related to a wide range of physically important phenomena from nonlinear transport in low-dimensional biological, polymeric, and condensed matter systems to electric pulse propagation in nonlinear transmission lines and light pulse propagation in tunnel- and nonlinearly coupled arrays of optical fibers. In doing so we have suggested the systematic analytical approach suitable for the needs of nonlinear physics in more than one spatial dimension and have studied the structure of simplest nonlinear excitations on two- and three-leg ladder lattices.

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