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DIPOLE–MONOPOLE CROSSOVER AND CHARGELESS HALF-MODE IN AN INTEGRABLE EXCITON–PHONON NONLINEAR DYNAMICAL SYSTEM ON A REGULAR ONE-DIMENSIONAL LATTICE

A new form of the integrable nonlinear exciton–phonon dynamical system characterized by two physically independent parameters is suggested. The system is settled along an infinite one-dimensional regular lattice, and it admits the semi-discrete Lax representation in terms of 3×3 auxiliary spectral and evolution matrices. The explicit analytic four-component solution to the system's dynamical equations found by means of the Darboux–Bäcklund dressing technique turns out to be of broken $\mathcal{PT}$-symmetry. Each component of the solution consists of two nonlinearly superposed traveling waves that inspires the dipole–monopole crossover for the equal values of two physically distinct spatial scaling parameters of the nonlinear wave packet. The phenomenon of the dipole–monopole alternative for the spatial distribution of pseudoexcitons is shown to initiate the partial splitting between the pseudoexcitonic and vibrational subsystems at the threshold point manifested by the complete elimination of one pseudoexcitonic component and the conversion of another pseudoexcitonic component into the pseudoexcitonic chargeless half-mode.

Keywords: nonlinear exciton–phonon system, Lax integrability, dipole–monopole crossover, threshold point, chargeless half-mode.

1. Introduction

The study of nonlinear excited states in the coupled electron–phonon or exciton–phonon systems has a long and celebrated history [1–13]. From the physical standpoint, such systems are important as the generants of soliton-like nonlinear waves [6–8, 11, 12] responsible for the robust charge and energy transport in the low-dimensional macromolecular objects of distinct physical origins. In this respect, they inspire a huge number of interesting and very sophisticated physico-mathematical problems.

Here, we will pay attention to some recent aspects of the exciton–phonon modeling based upon the development and investigation of integrable nonlinear exciton–phonon dynamical systems on one-dimensional lattices mimicking the long macromolecules. In particular, we will consider and analyze the peculiarities of symmetry broken solutions to the $\mathcal{PT}$-symmetrical exciton–phonon system

$$\dot{g}_+(n) = J\, g_+(n+1) \exp\left[q(n+1) - q(n)\right] - J\, g_+(n), \tag{1.1}$$

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$$\dot{g}_-(n) = J\,g_-(n) - J\,g_-(n-1)\exp\left[q(n) - q(n-1)\right], \tag{1.2}$$

$$\dot{p}(n) = \left[\Omega^2 - J\,g_+(n+1)g_-(n)\right]\exp\left[q(n+1) - q(n)\right] - \left[\Omega^2 - J\,g_+(n)g_-(n-1)\right]\exp\left[q(n) - q(n-1)\right], \tag{1.3}$$

$$\dot{q}(n) = p(n) \tag{1.4}$$

distinguished by two explicit physical parameters in contrast with the recently proposed one-parameter predecessor [14, 15]. Here, the two sets $g_+(n) \equiv g_+(n|\tau)$, $g_-(n) \equiv g_-(n|\tau)$ and $p(n) \equiv p(n|\tau)$, $q(n) \equiv q(n|\tau)$ of field functions are related to the subsystem of pseudoexcitons and to the Toda vibrational subsystem, respectively. The over-dot stands for the differentiation with respect to the dimensionless time τ. The spatial position of a lattice site is marked by the integer n running from minus infinity to plus infinity. The real-valued constant parameters J and Ω are responsible for the intersite resonant coupling in the subsystem of pseudoexcitons and for the intersite elasticity in the vibrational subsystem, respectively. In addition, the parameter J is seen to determine the coupling strength between the subsystems.

2. Basic Properties of the Nonlinear Exciton–Phonon System under Study

The semidiscrete (differential-difference) nonlinear system of interest (1.1)–(1.4) is proved to be integrable in the Lax sense, inasmuch as it admits the zero-curvature representation

$$\dot{L}(n|\lambda) = A(n+1|\lambda)L(n|\lambda) - L(n|\lambda)A(n|\lambda), \tag{2.1}$$

with the spectral and evolution matrices $L(n|\lambda)$ and $A(n|\lambda)$ specified by the formulas

$$L(n|\lambda) = \begin{pmatrix} \lambda + p(n) + g_+(n)g_-(n) & g_-(n)\Omega/\sqrt{-J} & \Omega\exp\left[+q(n)\right] \\ g_+(n)\Omega/\sqrt{-J} & -\Omega^2/J & 0 \\ -\Omega\exp\left[-q(n)\right] & 0 & 0 \end{pmatrix}, \tag{2.2}$$

$$A(n|\lambda) = \begin{pmatrix} 0 & 0 & -\Omega\exp\left[+q(n)\right] \\ 0 & -J & g_+(n)\exp\left[+q(n)\right]\sqrt{-J} \\ \Omega\exp\left[-q(n-1)\right] & -g_-(n-1)\exp\left[-q(n-1)\right]\sqrt{-J} & \lambda \end{pmatrix} \tag{2.3}$$

and the spectral parameter λ being time-independent.

Due to its complete integrability, the nonlinear semidiscrete system (1.1)–(1.4) possesses an infinite number of conserved quantities. Here, we list only the most important of them

$$H = \sum_{m=-\infty}^{\infty} p^2(m)/2 - \sum_{m=-\infty}^{\infty}\left[\Omega^2 - Jg_+(m)g_-(m)\right] + \sum_{m=-\infty}^{\infty}\left[\Omega^2 - Jg_+(m)g_-(m-1)\right] \times \exp\left[q(m) - q(m-1)\right], \tag{2.4}$$

$$P = \sum_{m=-\infty}^{\infty} p(m), \tag{2.5}$$

$$C = \sum_{m=-\infty}^{\infty} g_+(m)g_-(m) \tag{2.6}$$

serving for the system's Hamiltonian function H, for the total momentum of a vibrational subsystem P, and for the total charge of a pseudoexcitonic subsystem C, respectively.

In general, the local density $\rho(n) = g_+(n)g_-(n)$ is not obliged to be a positively or negatively determined quantity. Namely for this reason, we treat it as the charge density of pseudoexcitons.

3. Analysis of Four-Component Symmetry Broken Solution Relying upon the Property of Dipole–Monopole Alternative

The simplest nontrivial four-component solution to the coupled semidiscrete nonlinear dynamical system (1.1)–(1.4) found in the framework of the Darboux–Bäcklund dressing technique is given by the following analytic expressions:

$$g_+(n) = \frac{2\,g_+|\Omega|\,[\cosh(\nu)-\cosh(\mu)]\exp[\nu(n-y(\tau)+1/2)]}{|\Omega|\cosh[\mu(n-x(\tau)+1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)+1/2)]}, \tag{3.1}$$

$$g_-(n) = g_-\left\{1-\exp(-\nu)\,\frac{|\Omega|\cosh[\mu(n-x(\tau)+1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)+1/2)]}{|\Omega|\cosh[\mu(n-x(\tau)-1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)-1/2)]}\right\}, \tag{3.2}$$

$$p(n) = \sigma|\Omega|\,\frac{|\Omega|\cosh[\mu(n-x(\tau)-1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)-1/2)]}{|\Omega|\cosh[\mu(n-x(\tau)+1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)+1/2)]} -$$

$$-\,\sigma|\Omega|\,\frac{|\Omega|\cosh[\mu(n-x(\tau)-3/2)]+|g_+g_-|\exp[\nu(n-y(\tau)-3/2)]}{|\Omega|\cosh[\mu(n-x(\tau)-1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)-1/2)]}, \tag{3.3}$$

$$q(n) = q+\ln\left\{\frac{|\Omega|\cosh[\mu(n-x(\tau)+1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)+1/2)]}{|\Omega|\cosh[\mu(n-x(\tau)-1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)-1/2)]}\right\}. \tag{3.4}$$

Here, the real-valued parameter ν is related to the physical parameters J and Ω by the formula $\exp(\nu) = |\Omega/J|$, while the sign parameter σ is determined as $\sigma = -J/|J|$. The product g_+g_- of the real-valued parameters g_+ and g_- is assumed to satisfy the condition $g_+g_- = -\sigma|g_+g_-|$. The free localization parameter μ must be the real-valued one. At last, the running position coordinates $x(\tau)$ and $y(\tau)$ of nonlinearly superposed waves are specified by the formulas

$$\mu x(\tau) = \sigma\,\tau|\Omega|\sinh(\mu)+\mu x(0), \tag{3.5}$$

$$\nu y(\tau) = \sigma\tau|\Omega|\,[\cosh(\mu)-\exp(-\nu)]+\nu y(0). \tag{3.6}$$

In order to observe the phenomenon of dipole–monopole alternative in the above-written four-component solution (3.1)–(3.4), it is reasonable to consider the expression

$$g_+(n)g_-(n) = 4\,g_+g_-\,\Omega^2\,[\cosh(\mu)-\cosh(\nu)]\cosh(\mu/2)\cosh(\nu/2)\times$$
$$\times\frac{\exp[\nu(n-y(\tau))]\cosh[\mu(n-x(\tau))]}{|\Omega|\cosh[\mu(n-x(\tau)+1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)+1/2)]}\times$$
$$\times\frac{\tanh(\mu/2)\tanh[\mu(n-x(\tau))]-\tanh(\nu/2)}{|\Omega|\cosh[\mu(n-x(\tau)-1/2)]+|g_+g_-|\exp[\nu(n-y(\tau)-1/2)]} \tag{3.7}$$

for the product $g_+(n)g_-(n)$ of two pseudoexcitonic field components $g_+(n)$ and $g_-(n)$.

Having analyzed formula (3.7), we are able to reveal two principally distinct regimes of pseudoexcitonic dynamics separated by the threshold condition $|\mu| = |\nu|$. In particular, for $|\mu| > |\nu|$, the charge density of pseudoexcitons (3.7) strictly manifests itself as a sort of traveling dipole, inasmuch as the charge density changes its sign only in a single traveling spatial position, while the total charge of pseudoexcitons (2.6) is equal to zero. In contrast, for $|\mu| < |\nu|$, the sign of the charge density (3.7) is preserved on the whole infinite spatial interval, while the total charge (2.6) is of essentially nonzero value. As a result, for the critical relationship $|\mu| = |\nu|$ between the parameters μ and ν, the whole four-component symmetry broken solution (3.1)–(3.4) undergoes the crossover between the dipole and monopole scenarios of the charge density distribution.

In the very threshold point $|\mu| = |\nu|$, the $g_+(n)$-component (3.1) of the pseudoexcitonic subsystem is vanished, and the pseudoexcitonic mode is shrinked to a single $g_-(n)$-component (3.2). This survived component $g_-(n)$ can be referred to as the pseudoexcitonic chargeless half-mode, since it is unable to maintain a nonzero value of the charge density (3.7).

Moreover, the running position coordinates $x(\tau)$ and $y(\tau)$ calculated in the threshold point $|\mu| = |\nu|$ according to formulas (3.5) and (3.6) are characterized by the same velocity $v = \sigma\,(|\Omega|/\nu)\sinh(\nu)$. As a consequence, the simple manipulations with the expressions (3.3) and (3.4) for the components $p(n)$ and $q(n)$ of the vibrational subsystem renormalize them into the two-component solution typical of the standard Toda model [16, 17]. In other words, the evolution of the vibrational subsystem up to the mere renormalizing spatial shift turns out to be independent of the pseudoexcitonic chargeless half-mode, although the evolution of the pseudoxcitonic chargeless half-mode is still essentially dictated by the vibrational subsystem. This conclusion is also confirmed by the inspection of the basic semidiscrete nonlinear system (1.1)–(1.4) with the component $g_+(n)$ being compulsory eliminated.

4. Conclusion

The phenomenon of dipole–monopole alternative accompanied by the critical effect of the pseudoexcitonic chargeless half-mode exhibited by the suggested four-component analytic solution (3.1)–(3.4) is resulted from the specifically broken $\mathcal{PT}$-symmetry of this solution. Meanwhile, the dynamical equations of the basic nonlinear system (1.1)–(1.4) are the $\mathcal{PT}$-symmetric ones implying that the transformed field variables $\mathrm{g}_+(n) \equiv \mathrm{g}_+(n|\tau)$, $\mathrm{g}_-(n) \equiv \mathrm{g}_-(n|\tau)$, $\mathrm{p} \equiv \mathrm{p}(n|\tau)$, $\mathrm{q}(n) \equiv \mathrm{q}(n|\tau)$ defined by the equalities $\mathrm{g}_+(n|\tau) = g_-(-n|-\tau)$, $\mathrm{g}_-(n|\tau) = g_+(-n|-\tau)$, $\mathrm{p}(n|\tau) = +p(-n|-\tau)$, $\mathrm{q}(n|\tau) = -q(-n|-\tau)$ are checked to be governed by the same set of equations as the original nonlinear dynamical system (1.1)–(1.4).

In view of a generic $\mathcal{PT}$-symmetry of the nonlinear system under study (1.1)–(1.4), the already presented symmetry broken four-component solution (3.1)–(3.4) should inevitably induce its $\mathcal{PT}$-symmetry-broken partner solution. Evidently, such a $\mathcal{PT}$-symmetry-broken partner must demonstrate all physical features motivated by the phenomenon of dipole–monopole alternative.

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ДИПОЛЬНО–МОНОПОЛЬНИЙ ПЕРЕХІД
ТА БЕЗЗАРЯДОВА НАПІВМОДА В ІНТЕҐРОВНІЙ
ЕКСИТОН-ФОНОННІЙ НЕЛІНІЙНІЙ ДИНАМІЧНІЙ
СИСТЕМІ НА РЕГУЛЯРНІЙ ОДНОВИМІРНІЙ ҐРАТЦІ

Запропоновано нову форму інтеґровної екситон-фононної нелінійної динамічної системи з двома фізично незалежними параметрами. Система заселяє безмежну одновимірну регулярну ґратку і допускає напівдискретне представлення Лакса в термінах спектральної та еволюційної допоміжних матриць розміру 3 × 3. Явний аналітичний чотирикомпонентний розв'язок динамічних рівнянь системи, знайдений за допомоги техніки одягання Дарбу–Беклунда, є розв'язком з порушеною $\mathcal{PT}$-симетрією. Кожна з компонент розв'язку є певною нелінійною суперпозицією двох мандрівних хвиль, що зумовлює дипольно-монопольний перехід в системі за однакових значень двох фізично відмінних просторових масштабних параметрів нелінійного хвильового пакету. Показано, що явище дипольно-монопольної альтернативи в просторовому розподілі псевдоекситонів ініціює часткове розщеплення між псевдоекситонною і коливною підсистемами за критичного значення параметра локалізації. Це розщеплення полягає в повному вилученні однієї з псевдоекситонних компонент та перетворенні іншої псевдоекситонної компоненти у псевдоекситонну беззарядову напівмоду.

Ключові слова: нелінійна екситон-фононна система, Лаксова інтеґровність, дипольно–монопольний кросовер, критична точка, беззарядова напівмода.