Low Temperature Physics/Fizika Nizkikh Temperatur, 2021, vol. 47, No. 12, pp. 1186–1190

Coupling-managed criticality in nonlinear dynamics of an integrable exciton-phonon system on a one-dimensional lattice

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Received April 26, 2021, published online October 25, 2021

A one-dimensional nonlinear dynamical system of coupled intra-site excitations and lattice vibrations is studied. The system as a whole is shown to be integrable in the Lax sense and it admits the exact four-component analytical solution demonstrating the pronounced mutual influence between the interacting subsystems in the form of essentially nonlinear superposition of two principally distinct types of traveling waves. The interplay between the coupling strength and the parameter of localization causes the criticality of system's dynamics manifested as the dipole-monopole transition in the spatial distribution of intra-site excitations.

Keywords: exciton-phonon coupling, nonlinear integrable system, one-dimensional lattice, nonlinear wave packet, dipole-monopole transition.

1. Introduction

Since the pioneering works on the formation of polarons in ionic crystals [1–3] the consistent approaches to describe the effects of electron-phonon (or exciton-phonon) interaction in various condensed matter systems became the crucial idea of fundamental physical science. Such a type of interaction causes the Fröhlich–Peierls instability [4, 5] originating super-conducting states [4, 6] or charge-density waves [7–9] in quasi-one-dimensional metals [8, 9]. The similar sort of interaction is responsible for the formation of solitons in quasi-one-dimensional molecular structures [10–15] and charge-density packets in armchair silicene nanoribbons [16].

In general, the nontrivial physics of multi-component systems are usually manifested as essentially nonlinear effects supported by the strong coupling between the involved subsystems irrespective of their physical origins [17, 18]. This fact inspires the development of integrable multi-component models being able to grasp the most featured nonlinear effects in diverse physical systems.

However up to now, the exactly integrable nonlinear models dealing with the coupled exciton-phonon systems on a quasi-one-dimensional lattice have not jet been known. Recently we have tried to fill in this gap and suggested the semi-discrete integrable nonlinear model encompassing the subsystem of $\mathcal{PT}$-symmetric Dirac excitons and the subsystem of Toda lattice vibrations via their mutual interaction [19, 20].

In the present research we perform the linear analysis of this semi-discrete nonlinear integrable model elucidating the physical meaning of its field variables, and we describe the exact multi-component solution featuring the main nonlinear dynamical properties of the model.

2. Coupled system of Toda vibrations and Dirac excitons. Equations of motion, symmetry and linear analysis

Using the proper notations, the semi-discrete nonlinear integrable system of our interest [19, 20] is written as follows:

$$\dot{p}(n) = \left[1 + wg_+(n+1)g_-(n)\right]\exp\left[+q(n+1) - q(n)\right] - \left[1 + wg_+(n)g_-(n-1)\right]\exp\left[+q(n) - q(n-1)\right], \quad (1)$$

$$\dot{q}(n) = p(n), \quad (2)$$

$$\dot{g}_+(n) = wg_+(n) - wg_+(n+1)\exp\left[+q(n+1) - q(n)\right], \quad (3)$$

$$\dot{g}_-(n) = wg_-(n-1)\exp\left[+q(n) - q(n-1)\right] - wg_-(n). \quad (4)$$

Here the two sets $p(n) \equiv p(n\,|\,\tau)$, $q(n) \equiv q(n\,|\,\tau)$ and $g_+(n) \equiv g_+(n\,|\,\tau)$, $g_-(n) \equiv g_-(n\,|\,\tau)$ of field functions are related to the Toda vibrational subsystem and to the subsystem of Dirac excitons, respectively. The over-dot stands for the differentiation over 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 constant free parameter w determines the coupling strength between the subsystems.

The system under study (1)–(4) clearly demonstrates the symmetry under the space and time reversal ($\mathcal{PT}$-symmetry) implying that the transformed field functions $"p"(n) \equiv "p"(n|\tau)$, $"q"(n) \equiv "q"(n|\tau)$ and $"g"_+(n) \equiv "g"_+(n|\tau)$, $"g"_-(n) \equiv "g"_-(n|\tau)$ defined as

$$"p"(n|\tau) = +p(-n|-\tau), \tag{5}$$

$$"q"(n|\tau) = -q(-n|-\tau) \tag{6}$$

and

$$"g"_+(n|\tau) = g_-(-n|-\tau)\exp(+\alpha), \tag{7}$$

$$"g"_-(n|\tau) = g_+(-n|-\tau)\exp(-\alpha) \tag{8}$$

are governed by the same set of equations as that (1)–(4) for the original field functions $p(n)$, $q(n)$ and $g_+(n)$, $g_-(n)$. Here α is an arbitrary constant parameter.

The linear analysis of the system (1)–(4) based upon the low-amplitude harmonic traveling waves

$$q(n) = \varepsilon r \exp\left(ikn - i\omega\tau\right), \tag{9}$$

$$g_+(n) = \varepsilon h_+ \exp\left(ikn - i\omega\tau\right), \tag{10}$$

$$g_-(n) = \varepsilon h_- \exp\left(ikn - i\omega\tau\right) \tag{11}$$

yields two sorts of dispersion relations,

$$\omega(k) = 2\,|\sin(k/2)| \tag{12}$$

and

$$\omega_+(k) = w\sin(k) + 2i\,|w|\sin^2(k/2), \tag{13}$$

$$\omega_-(k) = w\sin(k) - 2i\,|w|\sin^2(k/2). \tag{14}$$

The first relation (12) is nothing but the dispersion relation for the acoustic vibrations in one-dimensional elastic chain [21, 22]. Another two relations (13) and (14) describe two submodes of exciton subsystem. The real parts $\mathrm{Re}\,\omega_+(k) = w\sin(k)$ and $\mathrm{Re}\,\omega_-(k) = w\sin(k)$ of these submodes coincide and demonstrate the dependence $w\sin(k)$ on quasi-momentum k typical of Dirac metamaterials [23–25]. Though the imaginary parts $\mathrm{Im}\,\omega_+(k) = +2|w|\sin^2(k/2)$ and $\mathrm{Im}\,\omega_-(k) = -2|w|\sin^2(k/2)$ of submodes (13) and (14) give rise to the gain and loss in mutually-reciprocal components $g_+(n)$ and $g_-(n)$ of the exciton subsystem, however the product $g_+(n)g_-(n)$ remains being balanced playing the part of some physically meaningful density, as it is usually required for physically motivated $\mathcal{PT}$-symmetric systems [26, 27].

3. Lax integrability and its outcomes

The nonlinear system of coupled Toda vibrations and Dirac excitons (1)–(4) is proved to be integrable in the Lax sense inasmuch as it admits zero-curvature representation [28–31]

$$\dot{L}(n|z) = A(n+1|z)L(n|z) - L(n|z)A(n|z) \tag{15}$$

serving as the compatibility condition for the auxiliary linear problem

$$X(n+1|z) = L(n|z)X(n|z), \tag{16}$$

$$\dot{X}(n|z) = A(n|z)X(n|z). \tag{17}$$

In the case of our system (1)–(4) the quantities $L(n|z)$, $A(n|z)$, $X(n|z)$ are taken as 3×3 square matrix-functions, where z is the free spectral parameter independent of time and coordinate. Having modified the notations of our previous articles [19, 20] we come to the expanded versions of spectral $L(n|z)$ and evolutionary $A(n|z)$ matrices given by formulas

$$L(n|z) = \begin{pmatrix} \lambda(z) + p(n) + g_+(n)g_-(n) & g_-(n)/\sqrt{w} & +\exp[+q(n)] \\ g_+(n)/\sqrt{w} & 1/w & 0 \\ -\exp[-q(n)] & 0 & 0 \end{pmatrix}, \tag{18}$$

$$A(n|z) = \begin{pmatrix} 0 & 0 & -\exp[+q(n)] \\ 0 & w & +\sqrt{w}g_+(n)\exp[+q(n)] \\ +\exp[-q(n-1)] & -\sqrt{w}g_-(n-1)\exp[-q(n-1)] & \lambda(z) \end{pmatrix}. \tag{19}$$

In view of its integrability the system under study (1)–(4) possesses an infinite hierarchy of conservation laws [20] obtainable in the framework of generalized direct recursive approach [32]. From the physical standpoint the most important conserved quantities are the Hamiltonian function H, the total momentum of Toda vibrations P and the total charge of Dirac excitons C defined, respectively, by the expressions:

$$H = \sum_{m=-\infty}^{\infty} p^2(m)/2$$

$$+\sum_{m=-\infty}^{\infty}\left[1+wg_+(m)g_-(m-1)\right]\exp\left[+q(m)-q(m-1)\right]$$

$$-\sum_{m=-\infty}^{\infty}\left[1+wg_+(m)g_-(m)\right], \qquad (20)$$

$$P = \sum_{m=-\infty}^{\infty} p(m), \qquad (21)$$

$$C = \sum_{m=-\infty}^{\infty} g_+(m)g_-(m). \qquad (22)$$

Taking into account the expression (20) for the Hamiltonian function H the nonlinear integrable system (1)–(4) must be treated as the dynamical system rewritable in the concise Hamiltonian form:

$$\dot{p}(n) = -\partial H/\partial q(n), \qquad (23)$$

$$\dot{q}(n) = +\partial H/\partial p(n), \qquad (24)$$

$$\dot{g}_+(n) = -\partial H/\partial g_-(n), \qquad (25)$$

$$\dot{g}_-(n) = +\partial H/\partial g_+(n). \qquad (26)$$

Thus, the two sets $p(n)$, $q(n)$ and $g_+(n)$, $g_-(n)$ of field functions acquire the sense of canonical field variables related to the Toda vibrational subsystem and to the subsystem of Dirac excitons, respectively.

The very existence of Lax representability (15)–(19) opens the door for searching the exact solutions to the suggested system (1)–(4) in the framework of one or another integration scheme. In the next Section we consider the simplest but rather instructive multi-component solution obtained by means of Darboux–Bäcklund dressing integration technique.

Fundamentals of the Darboux–Bäcklund dressing method as applied to multi-component semi-discrete integrable nonlinear systems are outlined in several recent papers [33–35].

4. Analytical four-component solution. Dipole and monopole scenarios of charge density distribution

Here, omitting all calculating details, we present the final analytical result for the four-component solution to our system (1)–(4) obtained in the framework of Darboux–Bäcklund dressing integration approach.

For this purpose it is convenient to parameterize the coupling strength w by formula

$$w = \sigma\exp(-\nu) \qquad (27)$$

with ν being an arbitrary real parameter and σ defined by the equality

$$\sigma^2 = 1. \qquad (28)$$

In addition, we introduce the notations

$$\mu x(\tau) = \sigma\tau\sinh(\mu) + \mu x(0), \qquad (29)$$

$$\nu y(\tau) = \sigma\tau\left[\cosh(\mu) - \exp(-\nu)\right] + \nu y(0) \qquad (30)$$

for the running position coordinates $x(\tau)$ and $y(\tau)$, and assign the condition

$$g_+g_- = -\sigma|g_+g_-| \qquad (31)$$

for the parameters g_+ and g_- to be valid. Here all involved parameters are assumed to be the real valued ones. Henceforth, each of two real parameters μ and ν can vary from minus to plus infinity.

Then, the nontrivial four-component solution to the coupled semi-discrete nonlinear dynamical system (1)–(4) are given by the following analytical expressions:

$$p(n) = \sigma\frac{\cosh\left[\mu(n-x(\tau)-1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-1/2)\right]}{\cosh\left[\mu(n-x(\tau)+1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)+1/2)\right]} - \sigma\frac{\cosh\left[\mu(n-x(\tau)-3/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-3/2)\right]}{\cosh\left[\mu(n-x(\tau)-1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-1/2)\right]}, \qquad (32)$$

$$q(n) = q + \ln\left\{\frac{\cosh\left[\mu(n-x(\tau)+1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)+1/2)\right]}{\cosh\left[\mu(n-x(\tau)-1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-1/2)\right]}\right\}, \qquad (33)$$

$$g_+(n) = \frac{2g_+\left[\cosh(\nu)-\cosh(\mu)\right]\exp\left[\nu(n-y(\tau)+1/2)\right]}{\cosh\left[\mu(n-x(\tau)+1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)+1/2)\right]}, \qquad (34)$$

$$g_-(n) = g_-\left\{1-\exp(-\nu)\frac{\cosh\left[\mu(n-x(\tau)+1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)+1/2)\right]}{\cosh\left[\mu(n-x(\tau)-1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-1/2)\right]}\right\}. \qquad (35)$$

At $\nu \neq 0$ the obtained four-component solution (32)–(35) clearly demonstrates the nonlinear superposition of two distinct types of traveling waves characterized by the two distinct velocities $\dot{x}(\tau) = (\sigma/\mu)\sinh(\mu)$ and $\dot{y}(\tau) = (\sigma/\nu) \times\left[\cosh(\mu) - \exp(-\nu)\right]$. As a consequence, the spatial configuration of each component becomes essentially dependent on time. The details of such an evolution are determined by the interplay between the parameter ν responsible for the strength of inter-subsystem coupling and the parameter μ regulating the spatial size of nonlinear wave packet. Only at $g_+ = 0$ and $g_- = 0$ the subsystem of Dirac excitons becomes completely unexcited and the whole dynamics are reduced to the dynamics typical of the Toda lattice [36, 37].

It is worth noticing, that the product of two Dirac amplitudes $g_+(n)g_-(n)$ is not obliged being positively defined function of its arguments n and τ. That is the reason why the quantity $g_+(n)g_-(n)$ should be treated as a sort of charge density rather than the density of excitons.

Let us illustrate this statement by analyzing the expression for $g_+(n)g_-(n)$ in the specific case of above-written four-component solution (32)–(35). Namely, we have

$$g_+(n)g_-(n) = 2\sigma|g_+g_-|\left[\cosh(\mu) - \cosh(\nu)\right]$$
$$\times\left\{\frac{\exp\left[\nu(n-y(\tau)+1/2)\right]}{\cosh\left[\mu(n-x(\tau)+1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)+1/2)\right]} - \frac{\exp\left[\nu(n-y(\tau)-1/2)\right]}{\cosh\left[\mu(n-x(\tau)-1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-1/2)\right]}\right\}. \qquad (36)$$

At $|\mu| > |\nu|$ each of two terms in curly brackets is finite and quickly tends to zero at both spatial infinities. Moreover, the functional forms of these two terms differ only by the primitive translation along a spatial coordinate. Inasmuch as the signs before these terms are distinct, the total charge C of Dirac excitons (22) calculated at $|\mu| > |\nu|$ on the examined charge density (36) is equal to zero. On the other hand, the same requirement $|\mu| > |\nu|$ ensures that the expression (36) for the charge density $g_+(n)g_-(n)$ changes its sign only in a single spatial coordinate position

$$\bar{n}(\tau) = x(\tau) + \frac{1}{\mu}\,\text{artanh}\left\{\frac{\tanh(\nu/2)}{\tanh(\mu/2)}\right\}. \qquad (37)$$

This coordinate position separates two oppositely charged parts of Dirac exciton wave packet, and it moves along the chain with the velocity $(\sigma/\mu)\sinh(\mu)$. Thus, at $|\mu| > |\nu|$ the charge density of Dirac excitons strictly manifests itself as a sort of traveling dipole. In contrast, at $|\mu| < |\nu|$ the sign of charge density (36) is preserved on the whole infinite spatial interval. As a consequence, at the critical relationship $|\mu| = |\nu|$ between parameters μ and ν the solution (32)–(35) undergoes the transition between the dipole and monopole scenarios of charge density distribution.

To substantiate the basic inferences concerning the physical features of the solution (36) obtained for the charge density $g_+(n)g_-(n)$ the alternative expression

$$g_+(n)g_-(n) = 4\sigma|g_+g_-|\left[\cosh(\mu) - \cosh(\nu)\right] \times \cosh(\mu/2)\cosh(\nu/2)$$
$$\times\frac{\exp\left[\nu(n-y(\tau))\right]\cosh\left[\mu(n-x(\tau))\right]}{\cosh\left[\mu(n-x(\tau)+1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)+1/2)\right]}$$
$$\times\frac{\tanh(\nu/2)-\tanh(\mu/2)\tanh\left[\mu(n-x(\tau))\right]}{\cosh\left[\mu(n-x(\tau)-1/2)\right]+|g_+g_-|\exp\left[\nu(n-y(\tau)-1/2)\right]} \qquad (38)$$

algebraically equivalent to the original one (36) is proved to be very useful.

5. Conclusion

In this article we have studied the main properties of a specific nonlinear exciton-phonon system on a regular one-dimensional lattice. Relying upon the system's integrability, we have managed to find rather representative four-component solution critical against the interplay between the coupling strength and the parameter of localization. The critical point (defined as $|\mu| = |\nu|$) separates two principally distinct dynamical regimes specified individually by the dipole and monopole distributions of charge density in the exciton subsystem. This unexpected result revealed on the simplest nontrivial solution would appear to prompt some new ideas for the future investigations of nonlinear physical systems characterized by the exciton-phonon interaction.

It is worth noticing, that despite the incontestable $\mathcal{PT}$-symmetry of considered nonlinear exciton-phonon system (1)–(4) the $\mathcal{PT}$-symmetry of suggested solution (32)–(35) is seen to be broken. Such a metamorphosis turns out to be rather typical phenomenon in other intrinsically $\mathcal{PT}$-symmetrical systems [27, 38–40]. According to recent experimental observations in $\mathcal{PT}$-symmetrical lasing devices the non-$\mathcal{PT}$-symmetric nonlinear modes are proved to be prospective for physical applications [38, 39].

Acknowledgement

The work has been supported by the National Academy of Sciences of Ukraine within the Project No. 0120U100855 (Properties of low-dimensional functional materials at nano-scales). The author is grateful to the Reviewer for the valuable comments directed to improve the text of the manuscript.

1. S. Pekar, *Zh. Eksp. Teor. Fiz.* **16**, 335 (1946).
2. L. D. Landau and S. I. Pekar, *Zh. Eksp. Teor. Fiz.* **18**, 419 (1948).
3. L. D. Landau and S. I. Pekar, *Ukr. J. Phys.* **53** (*Special Issue*), 71 (2008).
4. H. Fröhlich, *Proc. R. Soc. London A* **223**, 296 (1954).

5. R. E. Peierls, *Quantum theory of solids*, Clarendon Press, Oxford (1955).
6. A. A. Eremko, *Phys. Rev. B* **50**, 5160 (1994).
7. A. A. Eremko, *Phys. Rev. B* **46**, 3721 (1992).
8. S. van Smaalen, *Acta Cryst. A* **61**, 51 (2005).
9. J.-P. Pouget, *C. R. Phys.* **17**, 332 (2016).
10. A. S. Davydov and N. I. Kislukha, *Phys. Stat. Solidi B* **59**, 465 (1973).
11. A. S. Davydov, *Usp. Fiz. Nauk* **138**, 603 (1982).
12. A. S. Davydov, *Sov. Phys.–Uspekhi* **12**, 898 (1982).
13. A. C. Scott, *Phys. Rep.* **217**, 1 (1992).
14. J. Luo and B. M. A. G. Piette, *Eur. Phys. J. B* **90**, 155 (2017).
15. D. D. Georgiev and J. F. Glazebrook, *Physica E* **124**, 114332 (2020).
16. J. G. da Silva, B. G. Enders, G. M. e Silva, and A. L. de Almeida Fonseca, *Phys. Lett. A* **383**, 125954 (2019).
17. O. V. Charkina and M. M. Bogdan, *Fiz. Nizk. Temp.* **46**, 845 (2020) [*Low Temp. Phys.* **46**, 712 (2020)].
18. A. S. Kovalev and Y. E. Prilepskii, *Fiz. Nizk. Temp.* **46**, 1276 (2020) [*Low Temp. Phys.* **46**, 1083 (2020)].
19. O. O. Vakhnenko, *Ukr. J. Phys.* **58**, 1092 (2013).
20. O. O. Vakhnenko, *Phys. Lett. A* **384**, 126081 (2020).
21. A. S. Davydov, *Teoriya Tverdogo Tela* (*Theory of the Solid State*), Nauka, Moscow (1976).
22. A. S. Davydov, *Théorie du Solide*, Mir, Moscow (1980).
23. V. Yannopapas, *Int. J. Mod. Phys. B* **28**, 1441006 (2014).
24. B. Li, Zh. Li, J. Christensen, and K. T. Tan, *Appl. Phys. Lett.* **114**, 081906 (2019).
25. V. Apinyan and M. Sahakyan, *Rec. Progr. Mater.* **2**, 1 (2020).
26. A. Regensburger, C. Bersch, M.-A. Miri, G. Onishchukov, D. N. Christodoulides, and U. Peschel, *Nature* **488**, 167 (2012).
27. V. V. Konotop, J. Yang, and D. A. Zezyulin, *Rev. Mod. Phys.* **88**, 035002 (2016).
28. A. C. Newell, *Solitons in Mathematics and Physics*, SIAM Press, Philadelphia (1985).
29. L. A. Takhtadzhyan and L. D. Faddeyev, *Gamil'tonov Podkhod v Teorii Solitonov* (*Hamiltonian Approach to the Soliton Theory*), Nauka, Moscow (1986).
30. L. D. Faddeev and L. A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons*, Springer-Verlag, Berlin (1987).
31. G.-Z. Tu, *J. Phys. A: Math. Gen.* **22**, 2375 (1989).
32. O. O. Vakhnenko, *J. Nonlinear Math. Phys.* **18**, 401 (2011).
33. O. O. Vakhnenko, *J. Phys. Soc. Jpn.* **84**, 014003 (2015).
34. O. O. Vakhnenko, *Eur. Phys. J. Plus* **133**, 243 (2018).
35. O. O. Vakhnenko, *Wave Motion* **104**, 102745 (2021).
36. M. Toda, *Butsuri* **51**, 185 (1996).
37. M. Toda and K. Sogo, *J. Phys. A: Math. Theor.* **51**, 060201 (2018).
38. H. Hodaei, M.-A. Miri, M. Heinrich, D. N. Christodoulides, and M. Khajavikhan, *Science* **346**, 975 (2014).
39. R. El-Ganainy, K. G. Makris, M. Khajavikhan, Z. H. Musslimani, S. Rotter, and D. N. Christodoulides, *Nature Phys.* **14**, 11 (2018).
40. Y. Hanif and U. Saleem, *Nonlinear Dyn.* **98**, 233 (2019).

Взаємодіє-залежна критичність нелінійної динаміки інтеґровної екситон-фононної системи на одновимірній ґратці

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Розглянуто одновимірну нелінійну динамічну систему зв'язаних внутрішньовузлових збуджень та коливань ґратки. Показано, що система як ціле є інтеґровною в сенсі Лакса та допускає точний чотирикомпонентний аналітичний розв'язок, який вказує на значний взаємовплив між складовими підсистемами у вигляді суттєво нелінійної суперпозиції двох принципово відміних мандрівних хвиль. Зміна взаємовідношення між параметром зв'язку та параметром локалізації спричинює критичність динаміки системи і веде до переходу диполь-монополь у просторовому розподілі внутрішньовузлових збуджень.

Ключові слова: екситон-фононний зв'язок, нелінійна інтеґровна система, одновимірна ґратка, нелінійний хвильовий пакет, дипольно-монопольний перехід.