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POLARON DYNAMICS ON THE LATTICE WITH CUBIC NONLINEARITY. ACCURATE SOLUTION AND MULTIPEAKED POLARONS

Abstract.

Background. The feasible mechanism of charge transfer in quasi-one-dimensional systems is examined. Special interest to this problem emerged after the experimental discovery that the charge can travel dozens nanometers through the DNA chain with very high efficiency. It was found additionally that the charge transfer probability weakly depends on the lattice length and, moreover, occurs as a single-step coherent process. These properties open the possibilities for the usage of these and analogous systems as nanosized electroactive devices. The primary goal of the present paper is the theoretical and numerical feasibility study of the charge transfer in one-dimensional systems, representing the simplified DNA model, by means of polarons.

Materials and methods. The discrete model of one-dimensional classical oscillators with the cubic nonlinearity is utilized for the studying the problem, aimed at the elucidating the polaron mechanism of the charge transfer. The electron-phonon interaction is accounted in terms of the Su-Schriffer-Heeger (SSH) approximation. The referenced discrete model is reduced to two coupled nonlinear partial differential equations. One describes classical dynamical degrees of freedom. The other is the time-dependent Schrodinger equation for the electron wave function. The soliton-type solutions are derived at the definite relation between the model parameters (nonlinearity parameter α and the electron-phonon interaction χ). The numerical modeling shows the very high stability (polarons travel thousandth lattice sites without substantial changes in shape and amplitude). New polaron types with the envelope consisting of few (from 2 to 5) peaks are found in numerical simulation at larger parameter values. These properties are manifested for supersonic polarons with large amplitudes. The peaks existence is explained by the fact that the dynamically polaron is comprised by few solitons held together by the electron-phonon interaction. Multipeaked polarons are also very stable.

Results. The polaronic charge transfer mechanism is analyzed. The one-dimensional lattice model is used. The employed model describes the lattice dynamics classically. An accounting of the cubic nonlinearity in the neighboring particles interaction, allows to make the model more adequate with regard to original complex biological systems. Additionally, new qualitative properties are revealed. One is the existence of solitons and the role they are playing in the charge transfer. The wave function is reported in the adiabatic approximation, and the electron-phonon interaction is accounted in terms of the SSH approximation. Analytical solutions are derived for polarons on the nonlinear lattice. The solution shape (amplitude, width) is soliton-like and is governed by a single free parameter. Stable polarons with the envelope consisting of few peaks are found in numerical modelling.

Conclusions. It has been established that polarons on the lattice with the cubic nonlinearity are very stable and can participate in the charge and energy transfer in DNA and polypeptides. New types of multypeaked polarons are found. The dynamics is interpreted as the coupled state of few solitons hold together by the ekectron-phonon interaction.

Key words: quasi-one-dimensional systems, charge transfer, polarons, DNA chain, one-dimensional lattice model.

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ДИНАМИКА ПОЛЯРОНОВ НА РЕШЕТКЕ С КУБИЧЕСКОЙ НЕЛИНЕЙНОСТЬЮ. ТОЧНОЕ РЕШЕНИЕ И МНОГОПИКОВЫЕ ПОЛЯРОНЫ

Аннотация.

Актуальность и цели. Исследован возможный механизм переноса заряда в квазиодомерных системах. Особую актуальность этот вопрос приобрел после того, как экспериментально было показано, что носитель заряда с очень высокой эффективностью может проходить расстояние в несколько десятков нм по цепи ДНК. При этом вероятность переноса заряда очень слабо зависит от длины цепи, а сам перенос осуществляется как одностадийный когерентный процесс. Эти свойства открывают возможность для использования этих и подобных соединений в качестве наноразмерных электроактивных устройств. Целью настоящей работы является теоретическое и численное изучение переноса заряда посредством поляронов в одномерных системах, моделирующих цепь ДНК.

Материалы и методы. Для решения задачи о поляронном механизме переноса заряда в одномерных системах, имеющих регулярное строение, использована классическая модель нелинейных осцилляторов с кубической нелинейностью. Электрон-фононное взаимодействие учитывается в рамках приближения Су-Шриффера-Хигера (СШХ). Исходная дискретная модель в континуальном пределе сведена к двум связанным между собой нелинейным уравнениям в частных производных. Одно из них описывает классические динамические степени свободы, а второе есть уравнение Шредингера на волновую функцию электрона. При определенном соотношении между параметрами модели (параметр нелинейности потенциала α и параметр электрон-фононного взаимодействия χ) получено аналитическое решение солитонного типа. В численном моделировании показана высокая устойчивость полученных решений (поляроны проходят по цепи несколько тысяч постоянных решетки без изменения своей формы и амплитуды). При бóльших значениях параметров α и χ обнаружены новые типы поляронов, у которых огибающая не гладкая, а состоит из нескольких (от двух до пяти) пиков. Эти свойства проявляются для поляронов с большой амплитудой и скоростью превышающей скорость звука. Наличие пиков объяснено тем, что полярон образован несколькими солитонами, связанными между собой электрон-фононным взаимодействием. Эти поляроны также очень устойчивы, что подтверждено численным моделированием.

Результаты. Исследован механизм переноса заряда с помощью поляронов. Использована одномерная решеточная модель. Использованная модель описывает динамику решетки в классическом приближении. Учет кубической нелинейности в потенциале взаимодействия соседних частиц позволяет, во-первых, сделать модель более адекватной анализируемой физической системе; во-вторых, приводит к выявлению новых качественных свойств. Одно из таких свойств – существование солитонов и их роль в транспорте заряда. Волновая функция электрона описывается в адиабатическом приближении, а электрон-фононное взаимодействие учитывается в приближении СШХ. Получены аналитические решения для поляронов на нелинейной решетке. Вид этих решений (форма, амплитуда, скорость) солитоноподобный и определяется единственным свободным параметром. В численном моделировании обнаружены устойчивые поляроны, огибающая которых имеет несколько пиков.

Выводы. Показано, что поляроны на решетке с кубической нелинейностью очень устойчивы и могут переносить заряд и энергию в ДНК и полипептидах. Обнаружен новый тип многопиковых поляронов. Их динамика определяется солитонами, а сами солитоны удерживаются в связанном состоянии электрон-фононным взаимодействием.

Ключевые слова: квазиодомерные системы, перенос заряда, поляроны, цепь ДНК, одномерная решеточная модель.

Introduction

The Su – Schrieffer – Heeger (SSH) approximation aimed at the accounting the electron-phonon interaction is know since 1979–1980 [1, 2]. This approximation was initially applied to polyacetylene (PA) to describe the soliton-like (kink) excitations. Charge-density waves were found in the continuum version of PA [3]. The solution was obtained in the form of hyperbolic tangent kink order-parameter profile. Based on the same principles, the new solutions were found which were conventional strong-coupling polarons with spin 1/2 and charge $\pm e$ in the dimerized PA chain [4]. Though PA is rather special system being multielectron system with the dimerized ground state, the SSH model came into play in further investigations of low-dimensional molecular systems.

Polarons as "self-trapped" charge carriers can explain many effects associated with the charge transport in nonmetallic materials. Special interest arose after the effective charge transport over long distances (tenth nanometers) was discovered in synthetic DNA and polypeptides [5–12] (see also reviews [5, 13–15]). E. Conwell with colleagues was the first who applied the SSH approximation in an attempts to describe the charge transfer in DNA [16, 17] using the polaron paradigm. This line of research was further extensively studied [18–23].

Obtaining the analytical solution for polarons is of primary interest as it allows to make qualitative and quantitative assessments of different properties. Polaron solutions on the harmonic lattice in the SSH approximation were found recently [24–26]. The solution has the hyperbolic secants form typical for the soliton solution.

In the present paper the analytical solution for polarons on the anharmonic lattice is derived at special relation between parameters of lattice nonlinearity α and electron-phonon interaction χ. The solution is obtained in the continuum approximation for the large radius polaron. As the polaron radius is inversely proportional to the parameter χ, the continuum approximation implies that both parameters χ and α should be small. At larger parameters values and velocities acceding the sound velocity, a new family of multipeaked polarons is found in numerical modelling.

1. Exact solution in the continuum approximation

1.1. Theoretical model

We consider a lattice model of a molecular system (e.g. DNA duplex stack) consisting of N particles with free ends. A "particle" can represent a DNA base.

The hamiltonian consists of two contributions. One is classical lattice hamiltonian H_{lat} and next accounts for the electron--phonon interaction H_{eph}:

$$H = H_{lat} + H_{eph}, \tag{1}$$

where the lattice hamiltonian reads

$$H_{lat} = \frac{m}{2}\sum_{j=1}^{N}\dot{x}_j^2 + \frac{k}{2}\sum_{j=1}^{N-1}(x_{j+1} - x_j)^2 - \frac{\alpha}{3}\sum_{j=1}^{N-1}(x_{j+1} - x_j)^3 \tag{2}$$

and m,k, and α are mass of the particle, lattice rigidity and nonlinearity parameter, correspondingly; x_j is the deviation of i th particle from the equilibrium. The choice of this potential is explained by the fact that it represents the series expansion up to the third order of such potentials as Toda, Morse, Lennard-Jones and others.

The electron-phonon interaction is

$$H_{eph} =< \Psi^* \left| \hat{H}_{eph} \right| \Psi >, \tag{3}$$

where $\hat{H}_{eph}$ in the matrix representation reads

$$H_{eph} = \begin{pmatrix} e_1 & t_1 & 0 & \dots & 0 & 0 \\ t_1 & e_2 & t_2 & \dots & 0 & 0 \\ 0 & t_2 & e_3 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & e_{N-1} & t_{N-1} \\ 0 & 0 & 0 & \dots & t_{N-1} & e_N \end{pmatrix} \tag{4}$$

and the wave function Ψ is the N – vector: $\Psi \equiv \psi_1, \psi_2, \dots, \psi_N$. H_{eph} is the symmetrical tridiagonal matrix. On-site energies e_j stand on the main diagonal, and hopping integrals t_j – on secondary diagonals. Hopping integrals are expressed through the linear deviation of relative displacements from the equilibrium and are written in the SSH approximation:

$$t_j = -[t_0 - \chi(x_{j+1} - x_j)], \tag{5}$$

t_0 is the hopping integral at equilibrium and χ – parameter of electron-phonon interaction. If the lattice is comprised by equal particles then all on-site energies e_j are also equal and without loss of generality they can be put to zero, what defines the electron energy point of reference.

It is convenient to make the variables dimensionless. Three independent parameters, – mass m, rigidity coefficient k and energy t_0 in (1) and (5) are put numerically to unity. Then units of time and length can be made dimensionless:

$[t]=\sqrt{mk^{-1}}$ and $[L]=\sqrt{t_0 k^{-1}}$. Parameter α is also dimensionless: $\alpha \to \alpha/\sqrt{kt_0}$. If specific parameters values are chosen, e.g., $m=130$ a.m.u., $k=0.85$ eVÅ^{-2} and $t_0=0.3$ eV for DNA [18, 19, 22, 27], then the time unit is $[t]=0.13$ ps, and the length is measured in $[L]=0.59$ Å. The dimensionless values of other parameters for DNA: $\alpha=1.2$ and $\chi=1.1$. The same notations are preserved below for the dimensionless variables.

Other parameter values t_0 and χ in the SSH approximation are also used [28, 29], but the particular choice of numerical values does not significantly influence the final results. Two dimensionless equations in variables x_j and ψ_j are obtained from (1)–(5):

$$\ddot{x}_j = (x_{j-1} - 2x_j + x_{j+1}) + \alpha\left[(x_j - x_{j-1})^2 - (x_{j+1} - x_j)^2\right] +$$
$$+\chi\left[(\psi^*_{j-1}\psi_j - \psi^*_j\psi_{j+1}) + \text{c.c.}\right],$$
$$\dot{\psi}_j = -\frac{i}{\tilde{\hbar}}\left\{[1-\chi(x_j - x_{j-1})]\psi_{j-1} + [1-\chi(x_{j+1} - x_j)]\psi_{j+1}\right\}, \quad (6)$$

where the first equation is the Newtonian equation of motion, and the second -- time-dependent Schrödinger equation. $\tilde{\hbar}$ is the dimensionless Planck's constant. It is more convenient to use variables $q_j \equiv (x_{j+1} - x_j)$. Then system (6) transforms to

$$\ddot{q}_j = q_{j+1} - 2q_j + q_{j-1} - \alpha[(q_{j+1} - q_j)^2 - (q_j - q_{j-1})^2] -$$
$$-\chi\left[(\psi^*_{j+1}\psi_{j+2} - 2\psi^*_j\psi_{j+1} + \psi^*_{j-1}\psi_j) + \text{c.c.}\right], \quad (7)$$
$$\dot{\psi}_j = -\frac{i}{\tilde{\hbar}}\left[(1-\chi q_j)\psi_{j+1} + (1-\chi q_{j-1})\psi_{j-1}\right].$$

1.2. The continuum approximation

A general way of obtaining the solution of discrete equations like (7) is the usage of the continuum approximation. In the continuum approximation discrete variables are expanded into series:

$$q_{j\pm1} = q \pm a g_{j'} + \frac{a^2}{2!}q'' \pm \frac{a^3}{3!}q''' + \frac{a^4}{4!}q'''' \pm \ldots,$$
$$\psi_{j\pm1} = \psi \pm a\psi' + \frac{a^2}{2!}\psi'' \pm \ldots \quad (8)$$

where superscripts mean spatial derivatives of the corresponding orders and a is a dimensionless parameter of expansion (usually $a=1$). After the substitution of expansions (8) into (7) a system of partial differential equations (PDEs) is obtained:

$$q_{tt} = \left(q_{xx} + \frac{1}{12} q_{xxxx} \right) - \alpha \left(q^2 \right)_{xx} + 2\chi \left(\psi\psi^* \right)_{xx},$$

$$\psi_t = -\frac{i}{\tilde{\hbar}} [2(1 - \chi q)\psi + \psi_{xx}]. \quad (9)$$

1.3. Exactly integrable system and its solution

The PDEs system (9) does not belong to the class of exactly integrable equations and has no exact solution. But there exists the exactly integrable Zakharov –Shabat system [30]:

$$3z_{tt} = (z_{xxx} - 6zz_x)_x + 8|\varphi|^2_{xx},$$

$$i\varphi_t = \varphi_{xx} - z\varphi, \quad (10)$$

having multisoliton solutions. If $\alpha = 2\chi$ in (9) (coefficients before spatial derivatives in the RHS are equal) then after simple variable substitutions this system coincides with (10). And the one-soliton solution is [30]:

$$q(x,t) = -\frac{A}{\cosh^2[d(x - v_\text{p} t)]},$$

$$\psi(x,t) = \frac{B\exp[i(kx + \omega t)]}{\cosh[d(x - v_\text{p} t)]}, \quad (11)$$

where the polaron width $1/d$ and its velocity v_p are not yet defined; A and B are amplitudes of relative displacements and the wave function, correspondingly; $(kx + \omega t)$ is the wave function phase. x should be substituted by the discrete variable j for the solution on the lattice.

The substitution of (11) into (9) allows to find the relation between all parameters. The solution is one-parameteric. If the amplitude A is chosen as a free parameter, then all other parameters are expressed through A:

$$d = \sqrt{\alpha A} = \sqrt{2\chi A}, \quad B = \sqrt{d/2}, \quad (12)$$

with the velocity

$$v_\text{p} = \left(1 + \frac{2\alpha A}{3} - \sqrt{\frac{\chi^3}{A}} \right)^{1/2} \approx 1 + \frac{\alpha A}{3} - \frac{1}{2}\sqrt{\frac{\chi^3}{A}} \quad (13)$$

and the phase:

$$k = \tilde{\hbar} v_\text{p} / 2 \ll 1; \quad \omega = (2 + d^2 - k^2) / \tilde{\hbar} \gg 1 \quad (14)$$

(typically the dimensionless Planck's constant $\tilde{\hbar} \sim 10^{-2}$ with the chosen dimensionless parameters. The small value of $\tilde{\hbar}$ imposes the different time scales for specific dynamical and quantum times: the quantum time in (9) is $\sim 10^{-2}$ times smaller then the dynamical time. This fact should be taken into account in the join integration of system (7)).

The polaron velocity v_{p} varies in a wide range $0 \le v_{\text{p}} \lesssim 1.2$ (the upper velocity limit is defined by the lattice discreteness: the polaron becomes too narrow and its width $w \approx 1/d$ is comparable to the lattice period when the velocity exceeding the sound velocity $v_{snd} = 1$).

Note that if the electron-phonon interaction is absent, i.e. $\chi = 0$, then $q(x,t)$ in (11) is nothing else then soliton and its velocity (13) coincides with the velocity of soliton on the α-FPU lattice [31]. But if the lattice is harmonic, i.e. $\alpha = 0$ then the polaron velocity coincides with the velocity on the harmonic lattice [24, 26]. Thus, the expression for the polaron velocity is correct in two limiting cases.

1.4. Numerical test of polaron stability

The solution (11) with parameters (12), (13) is checked in numerical simulation. Fig. 1 shows the dependence of polaron velocity *vs.* its amplitude. The coincidence between the expression for the velocity (13) and numerical modelling is very good.

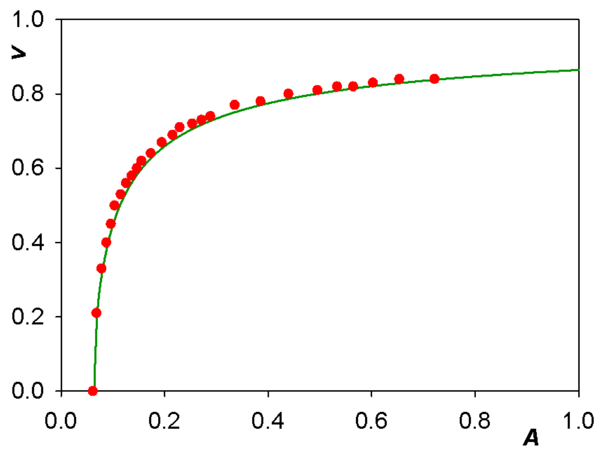

Fig. 1. (Color online) Dependence of the polaron velocity v vs. amplitude A. Solid line – formula (13) in the continuum approximation; filled circles – numerical integration of discrete equations (7)

Next figures shows the collision of polarons. Initial conditions are chosen according to (12)–(14) with parameters $A = 0.2$ and $A = 0.1$ for polarons 'X' and 'Z', correspondingly (Fig. 2).

This numerical experiment has no physical meaning as it does not take into account the Coulomb interaction. Its primary goal is the demonstration of high polaron stability and the accuracy of the solution. Traditionally, the elastic soliton collision in the soliton theory is believed to be the direct evidence of: *i*) soliton stability, and *ii*) that the solution belongs to the exactly integrable system.

2. Polarons at arbitrary parameters values: multipeaked polarons

The exact solution (11) is valid only if the relation $\alpha = 2\chi$ is valid and both parameters are small. In the general case these limitations are not fulfilled.

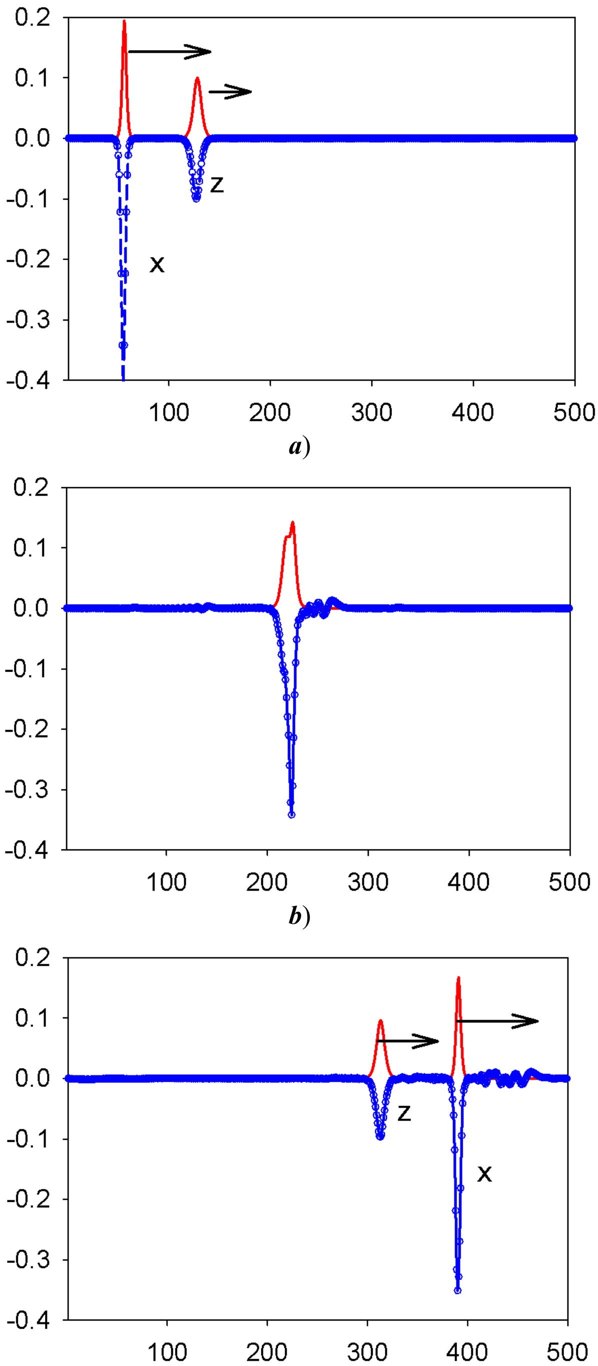

Fig. 2. (Color online) Collision of two of polarons: ***a*** – at time moment $t = 0$ polarons are centered at sites $j_0^X = 56$ and $j_0^Z = 128$. The initial velocity of the left polaron ‘X’ is larger than the velocity of the right polaron ‘Z’; ***b*** – polarons collision at $t = 200$; ***c*** – polarons after the collision at $t = 400$: polaron ‘X’ overruns more slower polaron ‘Z’. Positive values along the Y-axis – modulus of the wave function, negative -- relative displacements. Lattice with $N = 500$

For instance, the dimensionless parameters for DNA are $\alpha = 1.1$ and $\chi = 1.2$. Do polarons exist and are they stable at arbitrary parameters values? As the analytical solution is absent in this case, the numerical modelling is the only way to check this possibility. The parameter values $\alpha = 1.0$ and $\chi = 0.4$ are chosen for the more detailed analysis for definiteness. The results differ unessentially at other values of α and χ.

2.1. Standing and subsonic polarons

The exact solution at arbitrary parameters is unknown and the search of the solution is as follows. Initial conditions for the relative displacements are chosen according to (11). Initial amplitude A^0, velocity v_p^0 and the width parameter d^0 are arbitrary. The wave function is the eigenfunction of the matrix (4) with obtained values of hopping integrals $t_j = t_0 - \chi q_j$. It is hoped that if polaron does exist then it should self-organize from these initial conditions.

As a rule, these trial initial conditions are not the accurate solution, and it emits a "noise" which does not satisfy the conditions of the true solution. Gradually the polaron refines from all odds and acquires a stable shape and velocity.

The standing polaron obtained using this line is shown in Fig. 3.

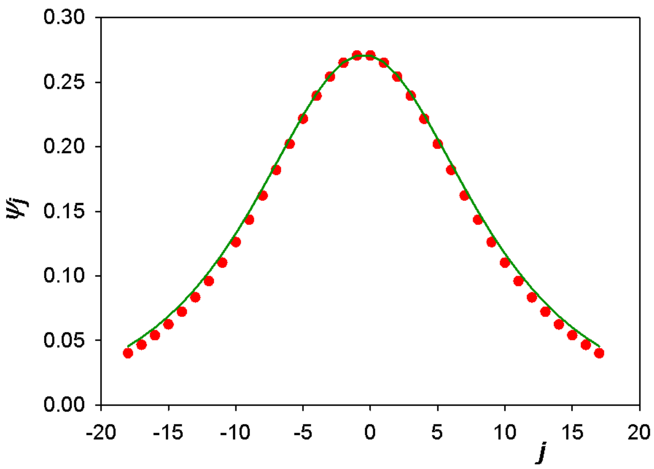

Fig. 3. (Color online) Calculated (circles) and fitting (solid line) for the wave function modulus. Parameters: $\alpha = 1.0$, $\chi = 0.4$

The relative displacements and the modulus of the wave function are approximated by the fitting

$$q_j = -\frac{A}{\cosh^2(dj)}, \; |\psi_j| = \frac{B}{\cosh^{\nu}(dj)} \qquad (15)$$

and $A = 0.055$, $B = 0.271$, $\nu = 1.23$ and $d = 0.129$. An existence of the fractional degree ν is not unusual. The best known analogy is the solution of the stationary Schrödinger equation with the potential $U(x) = -C sech^2(Dx)$. The solution has the general form $\psi(x) = B\cosh^{\nu}(bx)$. The exponent ν depends on values C and D in the potential $U(x)$ and can be fractional.

For what concerns the phase of the wave function, it depends on time $\propto \exp(-iE_{\text{p}}t/\tilde{\hbar})$ and is constant in the region where the polaron is located. The dependence of the wave function moduli on different sites j at different time instants is shown in Fig. 4.

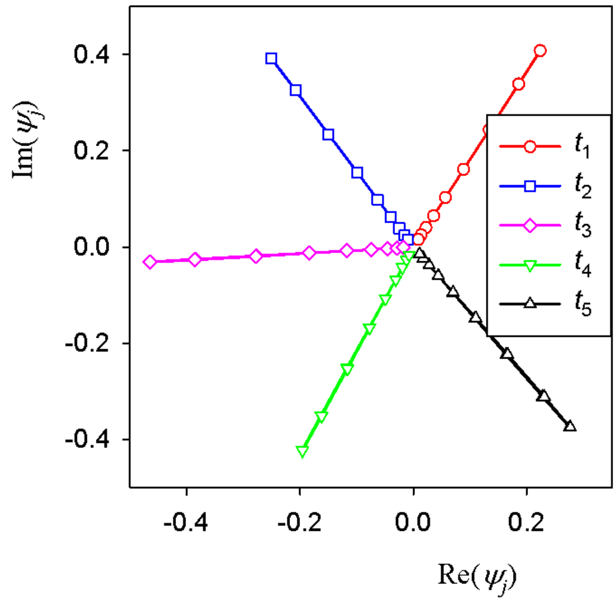

Fig. 4. (Color online) Real and imaginary parts of the wave function at different instants of time. Symbols correspond to different values of the wave function on different lattice site j (straight lines are shown to guide the eye). The time interval between consequent directions of the wave functions $\Delta t = t_2 - t_1 = t_3 - t_2 = \ldots = t_5 - t_4 = 6 \cdot 10^{-3}$. The wave function rotates anticlockwise. The total period of rotation $T \approx 3.6 \cdot 10^{-2}$

Straight lines $\tan\varphi = \mathrm{I}m(\psi_j)/\mathrm{Re}(\psi_j)$ ($j \subset$ polaron) at different instants of time demonstrate the constant values of the wave function phase φ. These data allow to find the contribution E_p determined by the electron-phonon interaction to the total polaron energy.

Polaron preserves its one-humped form up to velocity $v_{\text{p}} \lesssim v_{snd} = 1$. Subsonic polarons are very stable. They travel thousands lattice sites without noticeable changes in energy, shapes and velocity. Just as in the case with “analytical” polarons, “non-analytical” subsonic polarons with $\alpha = 1.0$ and $\chi = 0.4$ collides elastically. These issue can imply that there exists a stable solution which belongs to the (yet unknown) exactly integrable system.

2.2. Supersonic multipeaked polarons

When the polaron velocity exceeds the sound velocity, new polaron shapes with the envelope consisting of few peaks emerge. The modelling is done as follows: initial conditions for the relative displacements are chosen according to (11). As the relation between polaron parameters A^0, v_p^0 and d^0 is unknown, two of them (v_p^0 and d^0) are fixed. These values are chosen arbitrarily: $d^0 = 0.1, v_p^0 = 0.7$. The single variable parameter is the initial amplitude A^0. The initial wave function Ψ^0 is the eigenfunction of matrix (4) with the hopping integrals obtained from relative displacements $q(j, t = 0)$ (11).

As an example, the intermediate stage of the four-peaked polaron formation is shown in Fig. 5 at $A^0 = 0.6$. Few features of newly formed polaron should be outlined: 1) the polaron is identified by the 100% localized wave function. It self-organizes, increases the velocity up to stable $v_p = 1.14$; 2) relative displacements form an envelope consisting of four peaks; 3) the polaron is accompanied by at least five solitons arranged in the right order (the straight line in Fig. 4 shows the linear relation between the velocities and amplitudes specific to solitons). The polaron velocity lies between velocities of solitons S_1 and S_2.

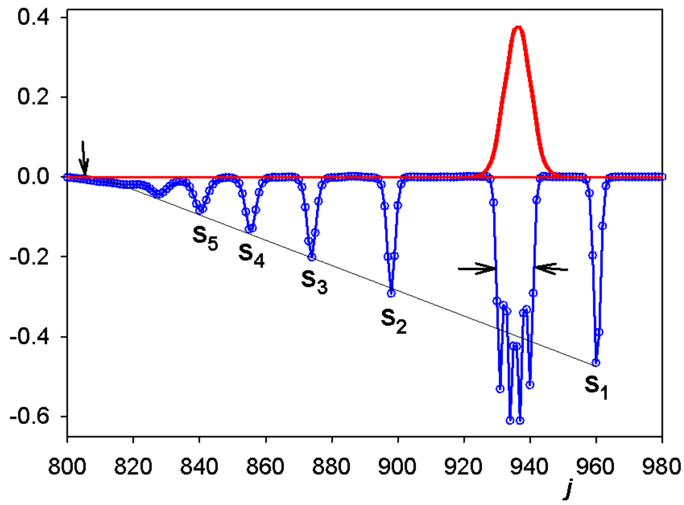

Fig. 5. (Color online) The result of the evolution of the initial excitation (see text) at $t = 800$. The formed four-peaked polaron is indicated by two horizontal arrows for clarity. There are also five solitons labelled by S_1, ..., S_5. Front edge of the sound propagation is shown by the vertical arrow. The steady state polaron velocity $v_p = 1.14$ increased relative to the initial value $v_p^0 = 0.7$. positive values – the wave function, negative – relative displacements

When the initial polaron amplitude A^0 changes, the number of peaks varies. Four examples for stable polarons with two, three, four and five peaks are shown in Fig. 6.

Number of peaks correlates with the steady polaron velocity. It is interesting to note that the change of peaks number looks like bifurcation – small variance of velocity results in dramatic change of peaks number (Fig. 7).

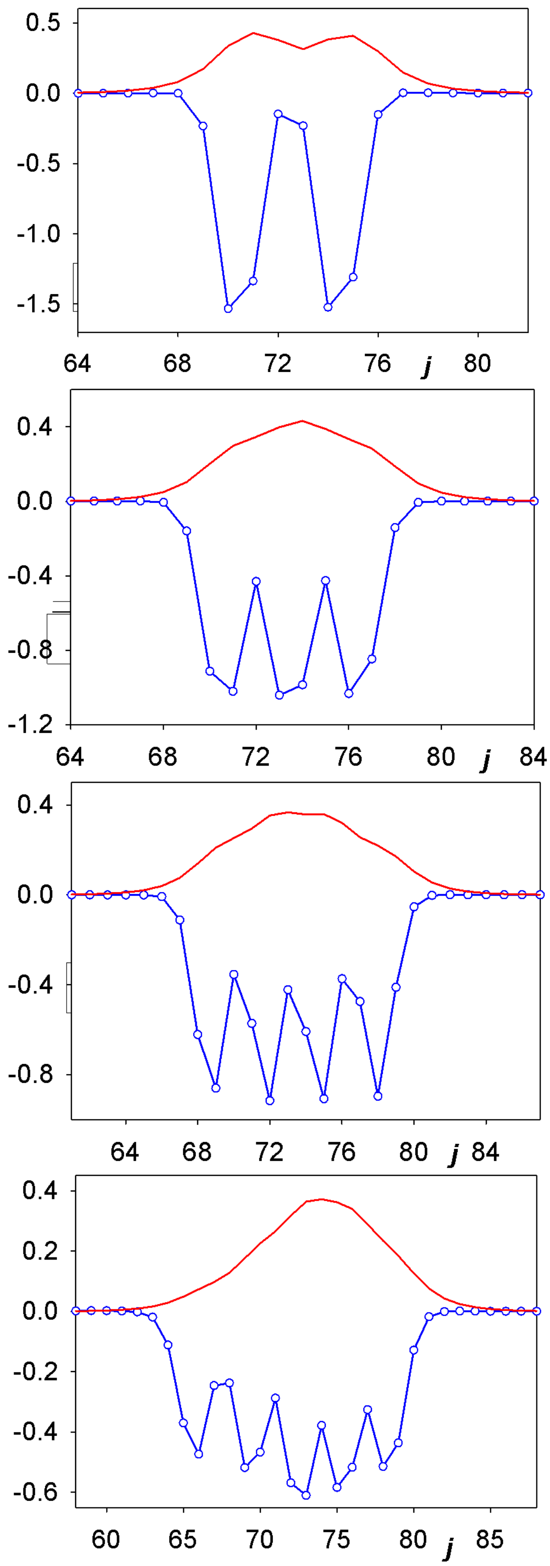

Fig. 6. (Color online) Polarons with two, three, four and five peaks. Snapshots are shown at $t = 900$

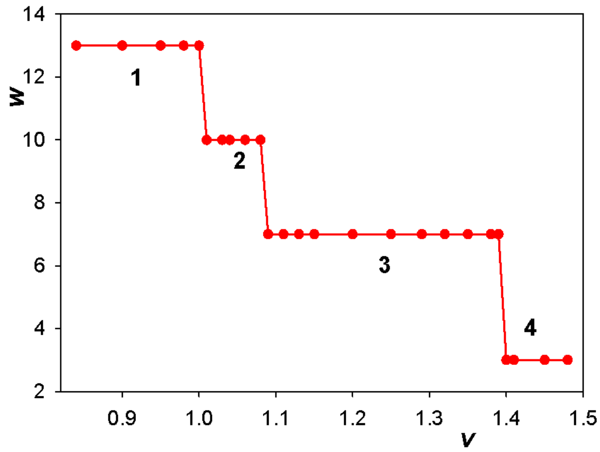

Fig. 7. (Color online) Polarons half-width w vs. steady velocities v.
Numbers indicate number of peaks. Horizontal lines show that the polaron widths and numbers of peaks are constant at some intervals of velocities

Multipeaked polarons were tested in collisions (Fig. 8). The collision is inelastic in contrast to the elastic collision of "analytical" polarons.

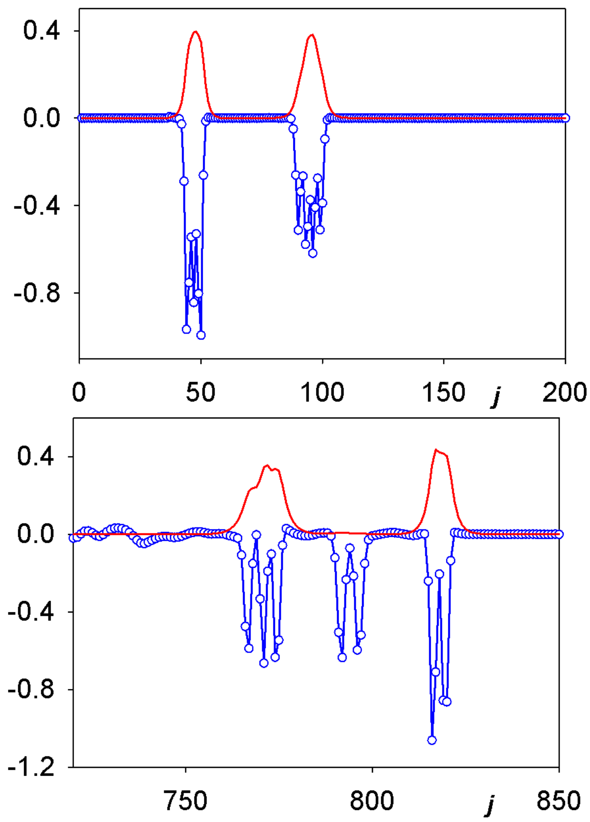

Fig. 8. (Color online) Inelastic collision of two multipeaked polarons.
Left panel: initial positions of polarons. The left three–peaked polaron has velocity larger then the right four-peaked polaron. Right panel: three-peaked and two-peaked polarons with two solitons in between after the collision at $t = 700$

An existence of peaks is of special interest. Evidently that the found multipeaked polarons do not belong to the well known polarobreathers (PBs) [32, 33] as the wave function is 100 % concentrated on polarons in contrast to PBs where the wave function is splitted between individual peaks.

The results presented in Fig. 8 can help in elucidating the peaks nature. Indeed, there are seven peaks in total before collision (three-peaked polaron collides with the four-peaked polaron). Seven "peaks" are also observed after the collision. Five peaks belong to polarons (three peaked plus two--peaked polarons). And two "peaks" are nothing else but solitons. Thus one can suspect that the multipeaked polaron might be comprised by solitons hold tightly by the electro-phonon interaction.

The following numerical experiment is performed to check this possibility. The KdV equation, which is the continuum approximation of the lattice with cubic nonlinearity, has the two-soliton solution. The solution for the relative displacements of two closely spaced polarons reads

$$q(x,t) = 1 + \exp\theta_1 + \exp\theta_2 + \left(\frac{a_1 - a_2}{a_1 + a_2}\right)\exp(\theta_1 + \theta_2), \qquad (16)$$

(where $\theta_i = a_i x - a_i^3 t, (i = 1,2)$ and $a_1 = 3.0, a_2 = 2.95$. The wave function is the eigenfunction of the matrix (4) with the hopping integrals employing relative displacements (16). After quick self-organization of this initial condition, the two-peaked polaron is formed (Fig. 9). It looks very much like the earlier found two-peaked polaron (Fig. 6).

Analogously, if three or four closely located solitons are "dressed up" by the wave function, the polaron is formed with the corresponding number of peaks. On contrary, if the polaron is "dressed down", i.e. the wave function is put to zero for a multipeaked polaron at any time instant, it decays into solitons. The number of solitons coincides with the number of peaks.

Conclusions

In conclusions we briefly summarize the main results. The detailed analysis is done for the polaron dynamics on the lattice with the cubic nonlinearity. The exact solution is obtained for the first time for large radius polarons when parameters of nonlinearity α and electron-phonon interaction χ are small, and comply with the requirements $\alpha = 2\chi$. The numerical modelling supports the high polaron stability. The elastic polaron collision (without considering the Coulomb interaction) is a strong evidence that the solution belongs to the class of exactly integrable systems. If the relation $\alpha = 2\chi$ is not valid, but both parameters are small, subsonic polarons are also very stable and collides elastically. This issue can point to the possibility that the solution also belongs to the (yet unknown) class of integrability.

When parameters α and χ become large (e.g. typical for DNA), new types of polarons is found. The envelope consists of few (up to five) peaks. The thorough analysis is done for the particular case when $\alpha = 1.0$ and $\chi = 0.4$. The multipeaked polaron are comprised of few solitons hold tightly together by the electron-phonon interaction.

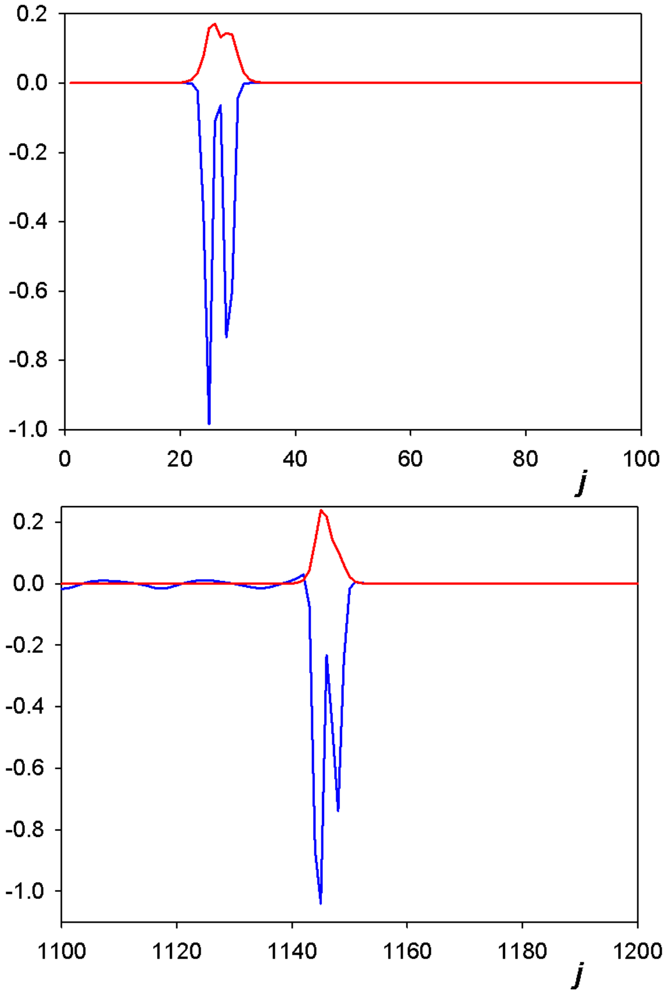

Fig. 9. (Color online) Formation of two-peaked polaron. Left panel:
initial condition – two-closely located solitons are "dressed up" by the wave function.
Right panel: snapshot of the initial condition evolution at $t = 1000$

The obtained results are valid in the wide range of parameters values. Necessary condition should be met that the electron-phonon interaction should be able to confine solitons together in the common potential well.

The most relevant investigations were done by M. Velarde with colleagues [34, 35]. They found the bounded state of soliton and electron, named solectron. But in contrast to our results, solectron has constant supersonic velocity coinciding with the velocity of a bare soliton.

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