Polarons on nonlinear lattice
in the Su–Schrieffer–Heeger approximation:
Exact solution and multipeaked polarons.

T.Yu. Astakhova, V.A. Kashin, V.N. Likhachev,
and G.A. Vinogradov

Emanuel Institute of Biochemical Physics, Russian Academy of Sciences,
Ul. Kosygina 4, Moscow 119991, Russian Federation
E-mail: *The corresponding author: gvin@deom.chph.ras.ru

Abstract.
We investigate the polaron dynamics on the nonlinear lattice with the cubic nonlinearity. The electron-phonon interaction is accounted in the Su-Schrieffer-Heeger approximation. An exact analytical solution is obtained in the continuum approximation at certain relation of parameters. The numerical simulation agrees with analytics very well. Moreover, colliding polarons recover their shapes and velocities after the elastic collision suggesting that the solution belongs to the exactly integrable system. When the continuum approximation is invalid (parameters of nonlinearity and electron-phonon interaction are not small), a new family of stable multipeaked polarons is found. These polarons are formed by the coupled solitons held together by the electron-phonon interaction.

1. Introduction
The Su–Schrieffer–Heeger (SSH) approximation aimed at the accounting the electron-phonon interaction is know since 1979 [1]. 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 [2-9] (see also reviews [2, 10-12]). E. Conwell with colleagues was the first who applied the SSH approximation in an attempts to describe the charge transfer in DNA [13, 14] using the polaron paradigm. This line of research was further extensively studied [15-20].

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 [21-23]. The solution has the hyperbolic secants form typical for the soliton solution.

In the present paper the analytical solution for polarons on the anharmonic α–Fermi-Pasta-Ulam (FPU) lattice is derived at special relation between parameters of lattice nonlinearity α and electron-phonon interaction χ, and when they are both small. At larger parameters values a new family of multipeaked polarons is found in numerical modelling.
2. Exact solution in the continuum approximation

2.1. Theoretical model

We consider a lattice model of a molecular system (e.g. DNA duplex stack) consisting of \( N \) particles with free ends. The dimensionless hamiltonian consists of two contributions. One is classical lattice hamiltonian \( H_{\text{lat}} \) and the other accounts for the electron-phonon interaction \( H_{\text{int}} : H = H_{\text{lat}} + H_{\text{int}} \), where the lattice hamiltonian reads

\[
H_{\text{lat}} = \frac{1}{2} \sum_{j=1}^{N} \tilde{\varepsilon}_j^2 + \frac{1}{2} \sum_{j=1}^{N-1} (x_{j+1} - x_j)^2 - \frac{\alpha}{3} \sum_{j=1}^{N-1} (x_{j+1} - x_j)^3
\]

and \( \alpha \) is the nonlinearity parameter. This \( \alpha \)-FPU potential is chosen because it represents the series expansion up to the third order of such potentials as Morse, Lennard-Jones etc. The electron-phonon interaction is

\[
H_{\text{int}} = \langle \Psi^* | \hat{H}_{\text{ep}} | \Psi \rangle
\]

where \( \hat{H}_{\text{ep}} \) in the matrix representation reads

\[
\hat{H}_{\text{ep}} = \begin{pmatrix}
e_1 & t_1 & \ldots & 0 & 0 \\
t_1 & e_2 & \ldots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & e_{N-1} & t_{N-1} \\
0 & 0 & \ldots & t_{N-1} & e_N
\end{pmatrix}
\]

and the wave function \( \Psi \) is the \( N \)-vector: \( \Psi = \psi_1, \psi_2, \ldots, \psi_N \). 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 means the electron energy point of reference.

It is more convenient to use variables \( q_j \equiv (x_{j+1} - x_j) \). Then the coupled system of Newton’s and Schrödinger equations arising from (1)–(3) reads

\[
\begin{align*}
\ddot{q}_j &= q_{j+1} - 2q_j + q_{j-1} - \alpha [(q_{j+1} - q_j)^2 - (q_j - q_{j-1})^2] - \\
&\quad \chi [(\psi^*_j \psi_{j+1} - 2\psi^*_j \psi_{j+2} + \psi^*_j \psi_{j-1}) + \text{c.c.}] \\
\dot{\psi}_j &= \frac{i}{\tilde{\hbar}} [(1 - \chi q_j) \psi_{j+1} + (1 - \chi q_{j-1}) \psi_{j-1}]
\end{align*}
\]

where \( \tilde{\hbar} \) is the dimensionless Planck’s constant (in molecular systems \( \tilde{\hbar} \sim 10^{-2} \)).

2.2. The continuum approximation and the solution.

A general way of obtaining the solution of discrete equations like (4) is the usage of the continuum approximation. In the continuum approximation discrete variables are expanded into series, e.g.

\[
q_{j \pm 1} = q \pm \alpha q_j^\prime + \frac{\alpha^2}{2!} q_j^\prime \prime \pm \frac{\alpha^3}{3!} q_j^\prime \prime \prime + \frac{\alpha^4}{4!} q_j^\prime \prime \prime \prime \pm \ldots
\]

where superscripts mean spatial derivatives of the corresponding orders and \( \alpha \) is a dimensionless parameter of expansion (\( \alpha = 1 \)). After the substitution of this expansions into (4) a system of partial differential equations (PDEs) is obtained:

\[
\begin{align*}
q_{tt} &= \left( q_{xx} + \frac{1}{12} q_{xxxx} \right) - \alpha (q^2)_{xx} + 2\chi (\psi^* \psi^\prime)_{xx} \\
\psi_t &= \frac{i}{\tilde{\hbar}} [2(1 - \chi q) \psi + \psi_{xx}]
\end{align*}
\]

The PDEs system (5) does not belong to the class of exactly integrable equations and has no an exact solution. But if \( \alpha = 2\chi \) then (5) coincides with the Zakharov-Shabat system [24] with the solution

\[
q(x, t) = -\frac{A}{\cosh^2[d(x - v_p t)]}; \quad \psi(x, t) = \frac{B \exp[i(kx + \omega t)]}{\cosh[d(x - v_p t)]}.
\]
Figure 1. (Color online). Collision of two of polarons. a) At time moment \( t = 0 \) polarons are centered at sites \( j_{0X}^0 = 56 \) and \( j_{0Z}^0 = 128 \). 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 – modulus of the wave function, negative – relative displacements. \( N = 500 \).

It can be shown that the soliton-like solution is one-parameteric and

\[
d = \sqrt{\alpha A} = \sqrt{2\chi A}, \quad B = \sqrt{d/2}, \quad v_p = \left(1 + \frac{2\alpha A}{3} - \sqrt{\frac{\chi^3}{A}}\right)^{1/2}
\]

with \( A \) being the free parameter. In the phase of the wave wave function: \( k \ll 1; \omega \gg 1 \).

Note that if the electron-phonon interaction is absent, i.e. \( \chi = 0 \), then \( q(x, t) \) is nothing else then soliton and its velocity coincides with the velocity of soliton on the \( \alpha \)-FPU lattice [25]. But if the lattice is harmonic, i.e. \( \alpha = 0 \) then the polaron velocity coincides with the velocity on the harmonic lattice [21, 23]. Thus, the expression for the polaron velocity is correct in two limiting cases.

2.3. Numerical test of polaron stability
The solution (6) is checked in numerical simulation on the lattice with parameters \( \chi = 0.2 \). The crucial experiment indicting the polaron stability is their collision. Figures 1 show the elastic collision of polarons. Initial conditions are chosen with parameters \( A = 0.2 \) and \( A = 0.1 \) for polarons ‘X’ and ‘Z’, correspondingly. 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. Moreover, this result points to the fact that PDEs (5) belong to the exactly integrable system.

3. Polaron at arbitrary parameters values: multipeaked polarons.
The exact solution (6) is valid only if \( \alpha = 2\chi \) and both parameters are small. In the general case these limitations are not fulfilled. 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 \( \alpha \) and \( \chi \).

When the polaron velocity is comparable with or exceeds the sound velocity, new polaron shapes with the envelope consisting of few peaks emerge. Four examples for stable polarons with two, three, four and five peaks are shown in Fig. 2
Multipeaked polarons were tested in collisions (see Fig. 3). The collision is inelastic in contrast to the elastic collision of “analytical” polarons. The results presented in Fig. 3 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 held tightly by the electro-phonon interaction.

The following numerical experiment is performed to check this possibility. The two-soliton solution of the KdV equation is

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

where \( \theta_i = a_i x - a_i^3 t, \ i = 1, 2 \) and \( a_i \) are parameters. The initial relative displacements are (8) with \( a_1 = 3.0 \) and \( a_2 = 2.95 \). The initial wave function is the eigenfunction of the matrix (3) with the hopping integrals employing relative displacements (8). After quick self-organization, the two-peaked polaron is formed (Fig. 4). It looks very much like the earlier found two-peaked polaron (Fig. 2).

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.
Figure 4. (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 $t = 1000$.

In conclusion: 1) we have found an exact solution for polarons on the $\alpha$-FPU lattice, and 2) found a new family of multipeaked polarons formed by the coupled solitons hold together by the electron-phonon interaction.

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