Polaron Dynamics on the Nonlinear Lattice in the Su–Schrieffer–Heeger Approximation. Exact and Approximate Solutions

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We investigate the polaron dynamics on the nonlinear lattice with the cubic nonlinearity in the tight-binding approximation. The electron–phonon interaction is accounted in the Su–Schrieffer–Heeger approximation. The system of nonlinear partial differential equations is derived in the continuum approximation. It has an exact solution at a special relation between parameters of lattice nonlinearity α and electron–phonon interaction χ. An approximate analytical solution is obtained at arbitrary parameters α and χ. Results of the numeric simulations are in a good agreement with the analytical predictions in both cases. The range of parameter values, where theoretical formulae are valid, is determined.

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1. Introduction

Polarons as "self-trapped" charge carriers can explain many effects associated with the charge transport in nonmetallic materials. Special interest was excited after the effective charge transport over long distances (tenth nanometers) was discovered in synthetic DNA and polypeptides [1–8] (see also reviews [1, 9–11]). E. Conwell with colleagues was probably the first who applied the SSH approximation in an attempts to describe the charge transfer in DNA [12, 13] using the polaron paradigm. This line of research was further extensively studied [14–21].

In the study of conductive polymers, organic semiconductors and molecular electronics, the tight-binding (TB) like models [22] are widely applied. The wave functions are based upon superposition of wave functions for isolated atoms located at each atomic site (the Wannier states). The interatomic matrix elements are represented as hopping parameters between neighboring sites. The TB approximation also demonstrated its efficiency in the study of charge transfer in non-metallic materials.

The Su–Schrieffer–Heeger (SSH) approximation aimed at the accounting the electron–phonon interaction is known since 1979–1980 [23, 24]. This approximation was initially applied to polyacetylene (PA) to describe the soliton-like (kink) excitations. 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 [25]. Though PA is a 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.

Obtaining the analytical solution for polarons is of primary interest as it allows qualitative and quantitative estimations of different properties. Few examples are known where the exact or approximate solutions are derived. One is the polaron solution on the harmonic lattice in SSH approximation [26–28]. It has the hyperbolic secant form typical for soliton solution. Similar in appearance solution is obtained for the Davydov–Scott model of charge transfer [29, 30]. The polaron solution is also derived for the Holstein model [31].

In the present paper the analytical solution for moving polarons on the anharmonic lattice is derived in SSH approximation 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 α and χ should be small. At larger parameters values an approximate analytical solution is also derived. The domain of the theory applicability is checked in numeric modeling.

2. Exact solution in the continuum approximation

2.1. Setting up the problem

We consider a lattice model of a molecular system (e.g. DNA chain) consisting of N particles in TB approximation. A "particle" can represent a DNA base. The Hamiltonian consists of two contributions. The one is classical

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lattice Hamiltonian $H_{\rm lat}$ and the other accounts for the electron–phonon interaction $H_{\rm int}$:

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

where the lattice Hamiltonian reads

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

and m, k and α are mass of the particle, lattice rigidity, and the nonlinearity parameter, correspondingly. The choice of this potential is explained by the fact that it represents the series expansion up to the second order of such "chemical" potentials as Morse, Lennard-Jones, Toda and others. The Hamiltonian of the electron–phonon interaction in the matrix representation is given by

$$H_{\rm int} = \begin{pmatrix} e_1 & t_1 & 0 & \dots & 0 & 0 \\ t_1 & e_2 & t_2 & \dots & 0 & 0 \\ 0 & t_2 & e_3 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & e_{N-1} & t_{N-1} \\ 0 & 0 & 0 & \dots & t_{N-1} & e_N \end{pmatrix}. \tag{3}$$

and the wave function is the N-vector $\Psi(t) = \psi_1(t), \psi_2(t), \dots, \psi_N(t)$. $H_{\rm int}$ is the symmetrical tridiagonal matrix. On-site energies e_j stand on the main diagonal and hopping transfer integrals t_j stand on secondary diagonals. Hopping integrals are expressed through the linear deviation of relative displacements from the equilibrium and in the SSH approximation are given by

$$t_j = -\left[t_0 - \chi\left(x_{j+1} - x_j\right)\right], \tag{4}$$

where t_0 is the hopping integral at equilibrium and χ is the parameter of electron–phonon interaction. The absolute value of the hopping integral increases if interparticle distance $(x_{j+1} - x_j)$ diminishes. If the lattice is homogeneous (comprised by equal particles) then all on-site energies e_j are equal and without loss of generality they can be set to zero, which means the electron energy point of reference.

It is convenient to make the variables dimensionless. We demonstrate the nondimensionalization by the example of DNA. Three independent parameters, e.g. mass m, rigidity coefficient k and energy t_0 in (1) and (4) can be chosen for said purpose. Typical values of these parameters are [17, 18, 21, 32]: $m = 130$ a.m.u. $= 2.16 \times 10^{-25}$ kg, $k = 0.85$ eV Å$^{-2} = 13.6$ kg s^{-2} and $t_0 = 0.3$ eV $= 4.8 \times 10^{-20}$ kg m^2 s^{-2}. All three values are set numerically to unity.

It is seen that the length unit can be constructed, using the dimensionality considerations, from parameters t_0 and k: $[L] = (t_0/k)^{1/2} = 0.59$ Å. Similarly, the time unit is the combination of m and k: $[t] = (m/k)^{1/2} = 0.13$ ps. These units are used as an example in the analysis of dimensionless DNA Hamiltonian (1). Other parameters values t_0 and χ in the SSH approximation are also used [33], but the particular choice of numerical values does not significantly influence the final results. Parameters α and χ are also reduced to the dimensionless form and $\alpha \approx 1.2$, $\chi \approx 1.1$ for DNA. The same notations for dimensionless parameters are used below.

The system of coupled dimensionless equations in variables x_j and ψ_j is obtained from (1)–(4):

$$\begin{aligned} \ddot{x}_j &= -\left(x_j - x_{j-1}\right) + \left(x_{j+1} - x_j\right) + \alpha\left[\left(x_j - x_{j-1}\right)^2 - \left(x_{j+1} - x_j\right)^2\right] - \chi\left(\left(\psi_{j-1}^*\psi_j - \psi_j^*\psi_{j+1}\right) + \left(\psi_{j-1}\psi_j^* - \psi_j\psi_{j+1}^*\right)\right) \\ \dot{\psi}_j &= -\frac{\mathrm{i}}{\tilde{\hbar}}\left\{\left[1 - \chi\left(x_j - x_{j-1}\right)\right]\psi_{j-1} + \left[1 - \chi\left(x_{j+1} - x_j\right)\right]\psi_{j+1}\right\}, \end{aligned} \tag{5}$$

where the first equation is the Newtonian equation, and the second is the time-dependent Schrödinger equation $\mathrm{i}\tilde{\hbar}\dot{\boldsymbol{\Psi}}(t) = H_{\rm int}\boldsymbol{\Psi}(t)$, where $\tilde{\hbar} \approx 1.7 \times 10^{-2}$ is the dimensionless Planck constant.

It is more convenient to rewrite system (5) in variables $q_j \equiv x_{j+1} - x_j$. Then system (5) transforms to

$$\begin{aligned} \ddot{q}_j &= q_{j+1} - 2q_j + q_{j-1} - \alpha\left[\left(q_{j+1} - q_j\right)^2 - \left(q_j - q_{j-1}\right)^2\right] - \chi\left(\left(\psi_{j+1}^*\psi_{j+2} - 2\psi_j^*\psi_{j+1} + \psi_{j-1}^*\psi_j\right) + \left(\psi_{j+1}\psi_{j+2}^* - 2\psi_j\psi_{j+1}^* + \psi_{j-1}\psi_j^*\right)\right) \\ \dot{\psi}_j &= -\frac{\mathrm{i}}{\tilde{\hbar}}\left[\left(1 - \chi q_j\right)\psi_{j+1} + \left(1 - \chi q_{j-1}\right)\psi_{j-1}\right]. \end{aligned} \tag{6}$$

This system is integrated using the fourth-order Runge–Kutta algorithm. In all cases the computational accuracy of the total energy and the wave function norm $< 10^{-5}$.

2.2. The continuum approximation

A common technique of deriving solution of discrete Eqs. (6) is the usage of the continuum approximation. In the continuum approximation discrete variables are expanded into series

$$\begin{aligned} q_{j\pm1} &= q \pm aq' + \frac{a^2}{2!}q'' \pm \frac{a^3}{3!}q''' + \frac{a^4}{4!}q'''' \pm \dots \\ \psi_{j\pm1} &= \psi \pm a\psi' + \frac{a^2}{2!}\psi'' \pm \dots, \end{aligned} \tag{7}$$

where primes mean spatial derivatives of the corresponding orders and a is a dimensionless parameter of expansion ($a = 1$). After the substitution of expansions (7) into (6) a system of partial differential equations (PDEs) is obtained

$$\begin{aligned} q_{tt} &= q_{xx} + \frac{1}{12}q_{xxxx} - \alpha\left(q^2\right)_{xx} + 2\chi\left(\psi\psi^*\right)_{xx} \\ \psi_t &= \frac{\mathrm{i}}{\tilde{\hbar}}\left[2\left(1 - \chi q\right)\psi + \psi_{xx}\right]. \end{aligned} \tag{8}$$

2.3. The particular solution of PDEs (8)

PDEs system (8) is not exactly integrable in general case. However, it reduced to integrable system when $\chi = 2\alpha$. In this case, it has a solution in the form of localized moving excitation

$$q(x,t) = -\frac{A}{\cosh^2\left((x-v_p t)/w\right)}$$

$$\psi(x,t) = \frac{B\exp\left(\mathrm{i}\left(kx+\omega t\right)\right)}{\cosh\left((x-v_p t)/w\right)}. \qquad (9)$$

Solution (9) has the form coinciding with the exact solution [26, 28] for the harmonic lattice, i.e. when $\alpha = 0$ in (8). The solution is specified by following parameters: w and v_p are the polaron width and velocity, A is an amplitude of relative displacements, B is an amplitude of the wave function, $(kx + \omega t)$ is the wave function phase.

Substitution of (9) into (8) with the wave function normalization condition $\int_{-\infty}^{+\infty} |\Psi(x)|^2\,\mathrm{d}x = 1$ results in the following relations between polaron parameters:

$$w = (2\alpha A)^{-1/2} = (\chi A)^{-1/2}, \quad B = (2w)^{-1/2},$$

$$v_p = \left(1 + \frac{2\alpha A}{3} - \sqrt{\frac{\chi^3}{A}}\right)^{1/2} \approx 1 + \frac{\alpha A}{3} - \frac{1}{2}\sqrt{\frac{\chi^3}{A}},$$

$$k = \tilde{\hbar} v_p/2 \ll 1, \quad \omega = \left(2 + w^{-2} - k^2\right)/\tilde{\hbar} \gg 1. \qquad (10)$$

Solution (10) is one-parametric, i.e. all parameters can be expressed through one free parameter. It is convenient to choose A as a free parameter. The substitution $x \to j$should be made in (9) to get the solution on the discrete lattice.

It worth noting that if the electron–phonon interaction is absent, i.e. $\chi = 0$, then $q(x,t)$ in (9) is nothing else but the soliton, and its velocity coincides with the velocity of soliton on the α-FPU lattice [34]. However, if the lattice is harmonic, i.e. $\alpha = 0$ then the polaron velocity coincides with the polaron velocity on the harmonic lattice [26, 28]. Thus, the expression for the polaron velocity (10) is correct in two limiting cases.

The dimensionless sound velocity is $v_{\mathrm{snd}} = 1$. Equation (10) shows that the lattice nonlinearity α increases the polaron velocity, and the electron–phonon interaction χ decreases the polaron velocity.

Both amplitudes A and B have lower limits for the standing polaron at $v_p = 0$: $A_{\min} \approx 0.063$ and $B_{\min} \approx 0.28$ when $\chi = 0.4$ and $\alpha = 0.2$. Amplitudes A and B increase with the growth of the polaron velocity.

2.4. Numeric test of the analytical solution

We analyze solution (9), (10) when $\chi = 2\alpha$ and the continuum approximation is valid. The solution accuracy is checked in numeric integration of discrete Eqs. (6).

We compare the results on the anharmonic lattice with the exact solutions on the harmonic lattice [28]. Figure 1a shows the dependence of the unmovable polaron amplitude A on χ for both harmonic and anharmonic lattices. One can see the good agreement between analytical and numeric results for the electron–phonon interaction $\chi \le 0.5$. It means that the continuum approximation is adequate in this range of χ values. For larger χ values polaron becomes narrower and its width w is comparable with the lattice period, and the continuum approximation is not valid. Moreover, Fig. 1a demonstrates that the difference between harmonic and anharmonic lattices is very small for $\chi < 0.5$. It is not surprising because the nonlinearity parameter is comparatively small ($\alpha \le 0.25$) and the overall dynamics does not differ significantly from the harmonic one.

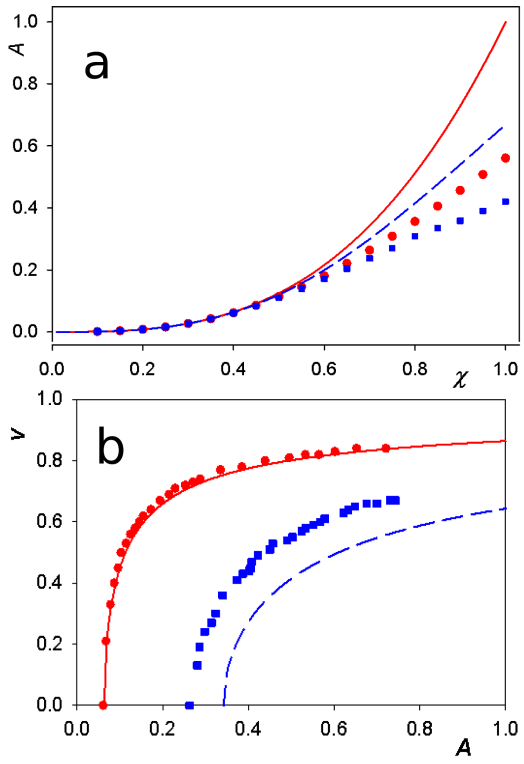

Fig. 1. a) The dependence of the unmovable polaron amplitude A on the parameter of electron-phonon interaction χ. Solid line and filled circles are the analytical expression and numeric results for the harmonic lattice. Dashed line and filled squares are the analytical expression and numeric results for the anharmonic lattice. b) The dependence of moving polaron velocity v_p on amplitude A for the anharmonic lattice. Solid line and filled circles are the analytical and numeric result for $\chi = 0.4$; dashed line and filled squares are analytical and numeric result for $\chi = 0.7$. (Recall that amplitude A is measured in the dimensionless units, unit length = 0.59 Å; unit velocity = unit length/unit time = 454 m/s).

The numeric test of solution (9) for moving polarons is shown in Fig. 1b where numeric and analytical results are compared for two values of χ. One can see an excellent agreement for $\chi = 0.4$, whereas analytical and numeric results differ noticeably for $\chi = 0.7$. However, numeric data demonstrate clearly pronounced relation between polaron amplitude and velocity. It indicates that there can exist a stable polaron solution on discrete lattice which is beyond the scope of our approximation.

Solution (9) is derived within two strict limitations: (i) the nonlinearity parameter α and the electron–phonon interaction χ are both small, and (ii) there fulfils the exact relation $\chi = 2\alpha$. In the general case it is not true. In

the next section we consider the case of arbitrary values α and χ.

3. An approximate solution at arbitrary parameter values χ and α

Numerical analysis shows that at arbitrary χ and α the wave function shape does not obey the simple hyperbolic cosine form and it can be better fitted by the fractional power of cosine. Thus, the trial solution is

$$q(x,t) = -\frac{A}{\cosh^2\left((x-v_p t)/w\right)}$$

$$\psi(x,t) = \frac{B\exp\left(\mathrm{i}\left(kx+\omega t\right)\right)}{\cosh^{\nu}\left((x-v_p t)/w\right)}, \qquad (11)$$

with fractional power $\nu > 1$; an expression for relative displacements coincides with (9). Broadly speaking, the fractional power in (11) is not surprising. It can be easily checked that the stationary Schrödinger equation with potential $U(x) = -C\cosh^{-2}(Dx)$ has solution $\psi(x) = B\cosh^{-\nu}(Dx)$, where ν depends on parameters C and D, and B is determined by the normalization condition $\int\limits_{-\infty}^{+\infty} |\Psi(x)|^2\,\mathrm{d}x = 1$. It is to be recalled that the trial solution similar to (11) for the self-trapped bell-shaped solutions in the Davydov–Scott model was used in [30]. Fraction power of hyperbolic secant was also used in variational analysis of moving breathers on the sine-Gordon lattice [35, 36]. Below we derive an approximate analytical solution of system (8) at arbitrary (but not too large) parameters χ and α using (11) as a trial solution.

Solution (11) exactly satisfies the second equation of system (8) and gives following relations between parameters:

$$A = \nu\left(\nu+1\right)/\left(2\chi w^2\right),$$

$$k = \tilde{\hbar} v_p/2 \ll 1, \quad \omega = \left(2 + w^{-2} - k^2\right)/\tilde{\hbar} \ll 1. \qquad (12)$$

It is convenient to make variable substitution $y = (x - v_p t)/w$. Then the first equation in (8) can be double integrated by y and the result is

$$\frac{g_1}{\cosh^2(y)} + \frac{g_2}{\cosh^4(y)} + \frac{g_3}{\cosh^{2\nu}(y)} = 0, \qquad (13)$$

where coefficients g_1, g_2, and g_3 are some combinations of parameters A, B, w, v_p, ν.

Afterwards the hyperbolic functions $\cosh^{-2}(y)$, $\cosh^{-4}(y)$, $\cosh^{-2\nu}(y)$ are expanded in series in terms of powers y up to the second order. Equating terms of zeroth and second powers by y, one gets two additional equations for the relation between parameters. The last, sixth, equation is obtained from the normalization condition of the wave function. As a result three additional equations for the relation between polaron parameters are derived which completely define the solution:

$$w^{-3} = \frac{(\nu-1)\,\chi^3}{4^{\nu-2} Z(\nu)\left[\alpha\nu^2\left(\nu+1\right)^2 - \chi\nu\left(\nu+1\right)\right]},$$

$$B^2 = \frac{1}{2^{2\nu-1} w Z(\nu)},$$

$$v_p^2 = 1 + \frac{Aw^{-2} - 6\left(2-\nu\right)\chi B^2}{3A}, \qquad (14)$$

where $Z(\nu) = \Gamma^2(\nu)/\Gamma(2\nu)$ and Γ is the gamma-function. Solution (11) is one-parametric, as previously, and ν is chosen as a free parameter. It can be easily checked that solutions (11), (12), (14) have the exact limit at $\nu \to 1$, when it converts into (9)–(10), which is equivalent to the case $\chi = 2\alpha$.

There exists one more particular exact solution at $\nu = 2$ (see (12) and (14)) with the following set of parameters:

$$A = 3/\left(\chi w^2\right), \quad B = \left(3/4w\right)^{1/2},$$

$$w^{-1} = \chi/\left(6\alpha - \chi\right)^{1/3} \quad v_p = \left[1 + 1/\left(3w^3\right)\right]^{1/2},$$

$$k = \tilde{\hbar} v_p/2, \quad \omega = \left(2 + w^{-2} - k^2\right)/\tilde{\hbar}. \qquad (15)$$

This solution corresponds to a single supersonic solution with fixed velocity, width and amplitude depending on χ and α.

Approximate solution with the trial functions (11) is checked in numerical simulations. Lattice parameters $\chi = \alpha = 0.4$ are chosen as an example. Initial conditions are specified by (11), (12), (14) with the free parameter $\nu = 1.4$. Figure 2 shows the evolution of the initial conditions. One can see that the polaron is very stable and holds the initial shape after travelling through ≈ 400 lattice sites.

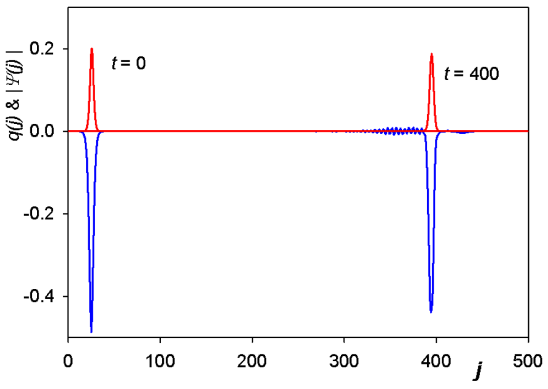

Fig. 2. Polaron evolution on the lattice with parameters $\chi = \alpha = 0.4$, $\nu = 1.4$, $N = 500$. Left polaron is defined by initial condition (11), (12), (14) at $t = 0$. Right polaron is the result of the evolution during $t = 400$. Positive values are modulus of wave function $|\psi(j)|$, negative values are relative lattice displacements q_j.

Next we compare analytical and numeric results. We investigate the lattice with fixed value of parameter of electron–phonon interaction $\chi = 0.4$. The anharmonicity parameter varies in range $\alpha \in [0.21{-}1.0]$. Value $\chi = 0.4$ is chosen as it is the largest value for which the continuum approximation is still valid. The lower value of $\alpha = 0.21$ is chosen as it is close to the exact solution (9), (10) for $\alpha = \chi/2 = 0.2$ (when $\nu = 1$). For smaller value of α ($\alpha < 0.2$) the difference between harmonic and anharmonic lattices vanishes. The choice of α upper value ($\alpha = 1.0$) is arbitrary.

Initial conditions are chosen according to (11), (12), (14) in the numeric simulation. Parameter ν varies in the range $\nu_{\min} < \nu \leq 2$, where $\nu_{\min}$ corresponds to the standing polaron ($v_p = 0$). The upper limit $\nu = 2$ is chosen as it corresponds to exact solution (15). There exist solutions (11), (12), (14) for $\nu > 2$.

The polaron parameters are analyzed after evolution time $t = 400$ at three different values of $\alpha = 0.21$, 0.4, 1.0; $\chi = 0.4$. Figure 3 shows the dependences of parameters (amplitude A and velocity v_p) vs. ν at different α. Solid lines show analytical dependences and symbols show numeric results. Recall that $\alpha = 0.2$ corresponds to the case of exact analytical solution (9), (10) which is a family of one-parametric solutions where $v_p \geq 0$, $A \geq A_{\min}$. Here $A_{\min}$ is determined from (10) for $v_p = 0$. This family of analytical solution for $\chi = 0.4$. $\alpha = 0.2$ corresponds to the vertical lines in Fig. 3 for $\chi = 0.4$, $\alpha = 0.2$, $A_{\min} \approx 0.06$. Figure 3 demonstrates that analytical and numeric results are in good agreement for amplitudes $A \leq 0.7$. For larger amplitudes the discreteness is essential and solutions (11), (12), (14) are not applicable.

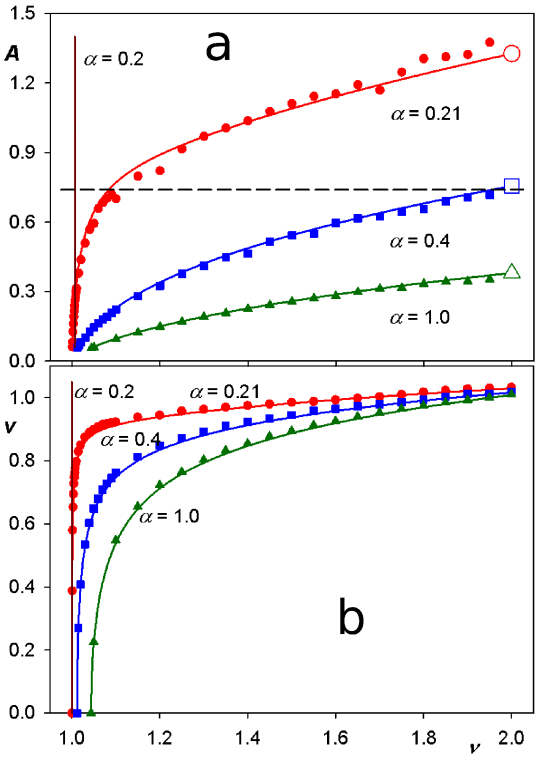

Fig. 3. The dependence of polaron parameters on ν after evolution time $t = 400$ at different α values. Solid lines are analytic expressions (12), (14), symbols are numeric results. a) Amplitude of relative displacements A vs. parameter ν. Dashed horizontal line shows the upper limit of the polaron amplitude $A \approx 0.7$, where numeric and analytical results coincide with high accuracy. b) Polaron velocities v_p vs. parameter ν.

4. Conclusions

In conclusions we briefly summarize the main results. The detailed analysis of the polaron dynamics on the lattice with cubic nonlinearity in the TB approximation is done. The exact solution is derived for large radius polarons when parameters of nonlinearity α and electron–phonon interaction χ are small, and comply with the requirements $\chi = 2\alpha$. The solution is soliton-like and is specified by a single free parameter, e.g. amplitude of relative displacements A. The numeric modeling demonstrates the high polaron stability and solution accuracy. If the relation $\chi = 2\alpha$ is not valid, but both parameters are small, an approximate solution is also derived.

Both the exact and approximate solutions are in good agreement with numeric simulations if the amplitude of relative displacements is not larger than a certain value $A_{\max}$ which depends on α and χ. For larger amplitudes the polaron width becomes too narrow and is comparable with the lattice period. In this case the continuum approximation within which the solutions are derived, becomes inapplicable.

The relation between numeric values of α and χ determine the solution type. If the nonlinearity is small then the solution behaves like the polaron on the harmonic lattice and the polaron is subsonic.

If electron–phonon interaction χ is small and nonlinearity α is sufficiently large, solitons are the dominant types of excitation on the α-FPU lattice. The wave function is trapped by the preliminary formed lattice deformation. The wave function adiabatically follows the soliton dynamics with the electron–phonon interaction negligibly influencing the polaron parameters. This scenario was investigated by Velarde with colleagues [37, 38] and they found the bounded state of soliton and electron, named solectron. However in contrast to our results, solectron has the supersonic velocity coinciding with the velocity of a bare soliton.

When parameters α and χ are comparable and are not small there is a competition between the non-linearity and electron–phonon interaction resulting in unusual solutions including multipeaked polarons [39].

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