Topological solitons in nondegenerate one-component chains

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The possibility of the existence of topological solitons in one-component chains with a nondegenerate potential of gradient type is proven. The existence and stability of the solitons are ensured by the competing nonlinear nearest-neighbor potential V_1 and parabolic second-nearest-neighbor potential V_2. Solitonic solutions have been found analytically for piecewise-parabolic V_1 and numerically for smoothened nearest-neighbor (NN) potential $V_{1,\delta}$. Numerical results for the soliton velocity and front width are in good agreement with analytical estimates. The solitons are shown to move at a unique velocity and actually maintain the constant profile as long as the NN potential is smooth enough. The impact of two solitons of different sign is inelastic and leads to their recombination. It is argued that the soliton propagation may constitute an elementary event of structural transformations in the chain.

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I. INTRODUCTION

Topological solitons are well known in continuum models of ordered one-dimensional atomic chains with onsite bistable (or multistable) degenerate potentials (ϕ^4, sine-Gordon models), when only homogeneous states with equal energies can exist [1–5]. Meanwhile, in many systems exhibiting structural transformations up to the appearance of random (glasslike) atomic configurations anharmonic potentials are of gradient type and have energetically nondegenerate equilibrium states [6–8].

Until recently it seemed that topological solitons in such situations were forbidden. The reason is that (i) contrary to the onsite potential, the multistable nature of gradient-type potentials is lost in continuum approximation, and (ii) nondegeneracy of the potential wells leads to the releasing or absorption of the energy during the transition from one well to another, which results in a contradiction with the condition of stationary propagation of topological solitons.

It turned out, however, that in multistable two-component (molecular) chains both of these difficulties might be overcome [6,7]. Namely, due to the presence of an optical branch of the IR spectrum, the gradient potential may be transformed under certain conditions to an onsite potential. If this takes place, topological solitons of a special type may exist in spite of nondegeneracy of the multistable potential. These solitons transfer the initial state into an intermediate one, which is in the attraction region of the final state, and may be responsible for structural transitions or chemical reactions in solids [7].

However, a question arises as to whether this is possible in one-component (atomic) chains. For a rather special case of a chain of particles with competing piecewise parabolic nearest-neighbor and harmonic next-nearest-neighbor potentials (Reichert-Schilling model [9,10]), a positive answer was obtained in Ref. [8]. Unfortunately, topological solitons in such a case turned out to be unstable.

In the present paper, the existence and stability of topological solitons in a nondegenerate one-component system with more realistic anharmonic potentials of gradient type, which may be obtained by smoothening a piecewise potential, are examined. The paper is organized as follows. In Sec. II, we outline the Reichert-Schilling model (RSM) and study the static features of background and solitonlike configurations. Section III is devoted to approximate analytical investigation of the dynamics of the RSM. In Sec. IV, we propose a numerical approach to the calculation of solitonic solutions for smooth potentials. A description of a transition between alternating and intermediate homogeneous states is given in Sec. V. Finally, in Sec. VI a molecular dynamics study of the existence and stability of topological solitons is presented.

II. STATIC REICHERT-SCHILLING MODEL

A. General theory

The RSM, first introduced in Ref. [9], is an infinite chain of identical classical particles with *anharmonic* and *competing* pair interactions along the chain up to the second neighbor leading to the following expression for the system's energy:

$$E=\sum_n V_1(u_{n+1}-u_n)+V_2(u_{n+2}-u_n)$$
$$=\sum_n V_1(w_n)+V_2(w_n+w_{n+1}), \qquad (1)$$

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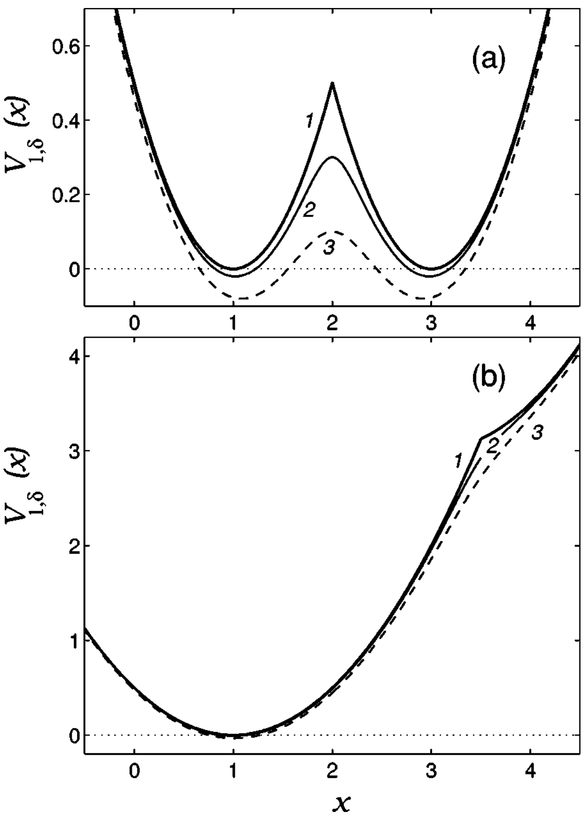

FIG. 1. The appearance of the NN interaction potential $V_{1,\delta}(x)$: $\alpha=1$, $a_1=1$, $a_2=3$; $\delta=0$, 0.2, 0.4 (curves 1, 2, 3) for (a) $c=2$ and (b) $c=3.5$.

where u_n are the particle positions and $w_n=u_{n+1}-u_n$ the bond lengths. Below we give a sketch of the principal results by Schilling *et al.* [9–11] in a slightly different yet equivalent notation [12].

The piecewise-parabolic nearest-neighbor (NN) potential is composed of two parabolas of the same curvature $C_1>0$,

$$V_1(x)=\frac{1}{2}C_1\{[x-a_+-a_-\sigma(x)]^2-[c-a_+-a_-\sigma(x)]^2\}, \tag{2}$$

$$a_\pm=\frac{1}{2}(a_2\pm a_1),\quad \sigma(x)=\text{sgn}(x-c)\in\{-1,+1\},$$

where a_1 and a_2 are positions of minima of the parabolas and c is the point where they are patched together [see Fig. 1(a), curve 1, and Fig. 1(b), curve 1]. The next-nearest-neighbor (NNN) interaction potential is harmonic,

$$V_2(x)=\frac{1}{2}C_2(x-b)^2,\quad C_2\neq 0.$$

The stationary equations

$$\frac{\partial E}{\partial w_n}=0,\quad n=0,\pm1,\pm2,\ldots \tag{3}$$

have been solved to yield a class of solutions:

$$w_n=r_0+y\sum_i \eta^{|i|}\sigma(w_{n+i}), \tag{4}$$

where

$$\eta=-\frac{1+2\alpha-\sqrt{1+4\alpha}}{2\alpha},\quad \alpha=C_2/C_1, \tag{5}$$

$$r_0=\frac{(1+\eta)^2a_+-2\eta b}{(1-\eta)^2},\quad y=a_-\frac{1+\eta}{1-\eta}. \tag{6}$$

Since w_n appears on both sides of Eq. (4), this is in fact a self-consistency equation for the stationary configurations $\{w_n\}$. Its solution may be found as follows: Replace $\{\sigma(w_n)\}$ on the right-hand side (rhs) by a sequence $\Sigma=\{\sigma_n\}$ of Ising-like variables $\sigma_n=\pm1$ and calculate the corresponding w_n. If for every k the self-consistency is satisfied, i.e., for every w_k calculated according to

$$w_n=r_0+yS_n,\quad S_n=\sum_i \eta^{|i|}\sigma_{n+i}, \tag{7}$$

we have $\sigma(w_k)\equiv\text{sgn}(w_k-c)=\sigma_k$, then this particular sequence $W=\{w_n\}$ is a solution to Eq. (4). Thus, every solution $\{w_n\}$ of the stationary equation (3) is in one-to-one correspondence with a binary Isinglike sequence $\{\sigma_n\}$.

Moreover, it was proven in Ref. [10] that if $a_->0$, $w_n>0$ for all n, and the geometric parameters of the potentials (a_1,a_2,b,c,η) lie in the range determined by inequality

$$|(1-\eta)^2c+2\eta b-(1+\eta)^2a_+|<(1+|\eta|)(1-3|\eta|)a_-, \tag{8}$$

then *each* sequence $\{\sigma_n\}$ gives a correct self-consistent solution $\{w_n\}$ of Eq. (3). Every such solution is related to a (locally) stable equilibrium configuration of the chain if $C_1>0$. At $C_1<0$ all the equilibrium configurations are unstable, and at $C_1=0$ the system splits into two independent harmonic sublattices.

Not only bond lengths but also the energy of the system in any equilibrium configuration may be expressed through Isinglike variables:

$$E(\Sigma)\equiv E(W(\Sigma))=E_0\sum_n 1-h\sum_n \sigma_n-\sum_{\substack{n,m\\ n\neq m}} J(n-m)\sigma_n\sigma_m, \tag{9}$$

where

$$E_0=-\frac{C_1}{2}\left\{\frac{1+\eta}{1-\eta}a_-^2+\frac{\eta}{(1-\eta)^2}b^2-\frac{4\eta}{(1-\eta)^2}ba_++c^2-2ca_++\left(\frac{1+\eta}{1-\eta}\right)^2a_+^2\right\}, \tag{10}$$

$$h=C_1a_-\frac{(1+\eta)^2a_+-(1-\eta)^2c-2\eta b}{(1-\eta)^2},$$

$$J(k)=J_0\eta^{|k|},\quad J_0=-\frac{C_1a_-^2}{2}\frac{1+\eta}{1-\eta}. \tag{11}$$

All the stationary configurations were found to be metastable for $C_1>0$ and $|\eta|<1$ (what is assumed below), and unstable for $C_1<0$.

Schilling *et al.* were interested primarily in the statistical properties of stationary chaotic configurations of the chain. They studied as well the chaotic chain motions, relaxation after quench, and dependence of the residual values of thermodynamic functions on the quench rate [13–17]. These properties are determined mostly by the kinetics of successive localized transformations of the chain. In contrast, we are going to study the solitonic (cooperative) motions in the RSM and RSM-like systems with smooth potential. This can only be done by approximate analytical or numerical techniques. Fortunately, certain limit cases of approximate solutions may be compared to exact results for the static RSM found on the basis of the general theory given above. For this purpose it is necessary to calculate the background and solitonlike static states of the system, which is the aim of the rest of this section.

B. Background states

Before we proceed, it is worth listing some useful identities that follow from Eq. (5):

$$\eta=-\frac{(\sqrt{1+4\alpha}-1)^2}{4\alpha},\quad \frac{1+\eta}{1-\eta}=\frac{1}{\sqrt{1+4\alpha}},$$

$$\frac{\eta}{(1-\eta)^2}=-\frac{\alpha}{1+4\alpha},\quad \frac{\eta}{1-\eta^2}=-\frac{\alpha}{\sqrt{1+4\alpha}}. \tag{12}$$

With their help, Eqs. (6) and (11) may be rewritten as

$$r_0=\frac{a_++2\alpha b}{1+4\alpha},\quad y=\frac{a_-}{\sqrt{1+4\alpha}}, \tag{13}$$

$$h=C_1a_-(r_0-c),\quad J_0=\frac{C_1a_-^2}{2\sqrt{1+4\alpha}}. \tag{14}$$

To find the background state we are only interested in the energy differences rather than their absolute values, so that we may omit the first sum in Eq. (9) to obtain

$$E'(\Sigma)=-\sum_n\sigma_n\left[h+J_0\sum_{i=1}^{\infty}\eta^i(\sigma_{n+i}+\sigma_{n-i})\right]. \tag{15}$$

Below we drop the prime on E. It is obvious that, depending on the signs of h and η, $E(\Sigma)$ can reach its minimum in either of the following cases: (i) $\sigma_n=+1$ for all n (such a configuration will be denoted below by $\Sigma=\{++\}$),

$$E=-\sum_n\left[h+2J_0\sum_{i=1}^{\infty}\eta^i\right]=\sum_n\mathcal{E}_{\mathrm{st}}^{\{++\}}, \tag{16}$$

where $\mathcal{E}_{\mathrm{st}}$ is the per site energy of a static configuration,

$$\mathcal{E}_{\mathrm{st}}^{\{++\}}=-h-2J_0\frac{\eta}{1-\eta}; \tag{17}$$

(ii) $\sigma_n=-1$ for all n (configuration $\{--\}$),

$$\mathcal{E}_{\mathrm{st}}^{\{--\}}=h-2J_0\frac{\eta}{1-\eta}; \tag{18}$$

(iii) $\sigma_{2k}=+1$, $\sigma_{2k+1}=-1$ (configuration $\{+-\}$ or equivalent configuration $\{-+\}$, which is obtained by enumeration shift); the second sum on the rhs of Eq. (9) vanishes, so that

$$\mathcal{E}_{\mathrm{st}}^{\{+-\}}=\mathcal{E}_{\mathrm{st}}^{\{-+\}}=-2J_0\sum_{i=1}^{\infty}(-\eta)^i=2J_0\frac{\eta}{1+\eta}. \tag{19}$$

To compare the energies of these states we subtract Eq. (19) from Eqs. (17) and (18) and transform the result with the help of Eqs. (12) and (14) to obtain

$$\mathcal{E}_{\mathrm{st}}^{\{++\}}-\mathcal{E}_{\mathrm{st}}^{\{+-\}}=-h-4J_0\frac{\eta}{1-\eta^2}=4e_0\alpha(1+\psi),$$

where

$$e_0=\frac{C_1a_-^2}{2(1+4\alpha)}=\frac{J_0}{\sqrt{1+4\alpha}},\quad \psi=-\frac{1+4\alpha}{2\alpha a_-}(r_0-c). \tag{20}$$

Similar derivations lead to

$$\mathcal{E}_{\mathrm{st}}^{\{--\}}-\mathcal{E}_{\mathrm{st}}^{\{+-\}}=4e_0\alpha(1-\psi).$$

One can easily see that $\{+-\}$ is the ground state if $\alpha>0$, $|\psi|<1$. If these conditions are not simultaneously satisfied, then either $\{++\}$ ($h>0$, i.e., $\alpha\psi<0$) or $\{--\}$ ($\alpha\psi>0$) is the ground state of the system.

It is of fundamental importance that the ground state with alternating bond lengths arises in the system with no extrinsic difference between these bonds. This is due to the effective long-range interaction along the chain: although the explicit pair interaction extends only to the second neighbor of the given particle, it may be seen from Eqs. (4) and (9) that every particle ''feels'' the influence of all other particles in the chain, the effective radius of interaction being inversely proportional to $(-\ln|\eta|)$. Such a feature suggests considering the states $\{+-\}$ and $\{-+\}$ as homogeneous states with double period, or *alternating uniform states* (AUS's). In contrast, configurations $\{++\}$ and $\{--\}$ will be referred to as *simple uniform states* (SUS's). This approach will enable us to reveal cooperative processes in *atomic* crystals.

We will denote by $\{\sigma_1\sigma_2\}$ such states that $\sigma(w_{2k})=\sigma_1$, $\sigma(w_{2k+1})=\sigma_2$ for all k. The intermolecular distances w_{2k} for uniform states will be denoted by r_s^+ for $\{++\}$, r_s^- for

$\{--\}$, r_a^+ for $\{+-\}$, and r_a^- for $\{-+\}$. In particular, we obtain for $\Sigma=\{++\}$ with the aid of Eq. (7),

$$S_n=-1+2\sum_{i=0}^{\infty}\eta^i=\frac{1+\eta}{1-\eta}=\frac{1}{\sqrt{1+4\alpha}}; \tag{21}$$

therefore

$$r_s^+=r_0+a_-/(1+4\alpha). \tag{22}$$

By analogy, we find that

$$r_s^-=r_0-a_-/(1+4\alpha), \quad r_a^{\pm}=r_0\pm a_-. \tag{23}$$

Equations (22) and (23) may be generalized as follows:

$$r(\{\sigma_1\sigma_2\})=r_0+a_-[\sigma_1+2\alpha(\sigma_1-\sigma_2)]/(1+4\alpha), \tag{24}$$

where $\sigma_i=\pm 1$. It is easy to see that $w_{2k+1}=w_{2k}$ for SUS's, while $w_{2k+1}=2r_0-w_{2k}$ for AUS's.

Thus, in the RSM under certain conditions every bond may either be "compressed" $[\sigma(w_j)\equiv\mathrm{sgn}(w_j-c)=-1]$ or "stretched" $[\sigma(w_j)=+1]$. The ground-state configuration is chosen by the model parameters among uniformly compressed ($\{--\}$), uniformly stretched ($\{++\}$), and alternating ($\{+-\}$ or $\{-+\}$) configurations. The RSM in alternating configurations may be considered as a uniform chain of diatomic molecules with constant intramolecular, w_{2k}, and intermolecular, w_{2k+1}, distances.

C. Solitonlike states

Among the whole variety of nonuniform states $\{\sigma_n\}$ we now choose for further study the simplest block-copolymer-like states, i.e., states of which each semi-infinite part of the chain, $\{\sigma_n|n<0\}$ and $\{\sigma_n|n\geqslant 0\}$, is in one of the homogenious states described above. We will denote by $\Sigma=\{\sigma_1\sigma_2|\sigma_3\sigma_4\}$ such states in which

$$\sigma_{2k}=\begin{cases}\sigma_1, & n<0,\\ \sigma_3, & n\geqslant 0;\end{cases}\quad \sigma_{2k+1}=\begin{cases}\sigma_2, & n<0,\\ \sigma_4, & n\geqslant 0;\end{cases} \tag{25}$$

we assume that $\{\sigma_1\sigma_2\}\not\equiv\{\sigma_3\sigma_4\}$. Substitution of Eq. (25) into Eq. (7) for different configurations yields the following results for $n\geqslant 0$: for (a) $\{--|++\}$, (b) $\{+-|++\}$, and (c) $\{-+|+-\}$, respectively,

$$S_n=\frac{1+\eta}{1-\eta}-\frac{2\eta^{n+1}}{1-\eta}, \quad S_{-n}=-S_{n-1}, \tag{26a}$$

$$S_n=\frac{1+\eta}{1-\eta}-\frac{2\eta^{n+1}}{1-\eta^2}, \quad S_{-n}=(-1)^n\frac{1-\eta}{1+\eta}+\frac{2\eta^{n+1}}{1-\eta^2}, \tag{26b}$$

$$S_n=(-1)^n\frac{1-\eta}{1+\eta}+\frac{2\eta^{n+1}}{1+\eta}, \quad S_{-n}=S_{n-1}. \tag{26c}$$

All other configurations of this kind may be reduced to those listed above by the following transformations: (i) changing all $\sigma_n\rightarrow-\sigma_n$, which leads to the change of sign in all S_n; (ii) turning the chain around the "block boundary," $n\rightarrow-(n+1)$; (iii) shifting the enumeration by 1, $n\rightarrow n\pm 1$.

Particle positions may be found as follows:

$$u_n=u_{n-1}+w_{n-1}=\cdots=u_0+\sum_{k=0}^{n-1}w_k$$
$$=u_0+nr_0+y\sum_{k=0}^{n-1}S_k, \quad n>0, \tag{27}$$

$$u_n=u_{n+1}-w_n=\cdots=u_0-\sum_{k=n}^{-1}w_k=u_0+nr_0-y\sum_{k=n}^{-1}S_k,$$
$$n<0. \tag{28}$$

Let us consider the RSM as a "molecular" chain consisting of diatomic "molecules" $[\sigma_{2k}\sigma_{2k+1}]$ and introduce molecular variables, mass center coordinate χ_k, and deformation ϕ_k according to

$$\chi_k=(u_{2k+1}+u_{2k})/2, \quad \phi_k=(u_{2k+1}-u_{2k})/2=w_{2k}/2. \tag{29}$$

With the help of Eqs. (26), (27), and (28) we find for $\Sigma=\{--|++\}$,

$$u_n=u_0+n\left(r_0+\mathrm{sgn}(n)\frac{a_-}{1+4\alpha}\right)-2a_-\frac{\eta(1+\eta)(1-\eta^{|n|})}{(1-\eta)^3},$$

$$\chi_k=u_0+\left(2k+\frac{1}{2}\right)\left(r_0+\mathrm{sgn}(k)\frac{a_-}{1+4\alpha}\right)$$
$$-a_-\frac{\eta(1+\eta)(2-\eta^{|2k|}-\eta^{|2k+1|})}{(1-\eta)^3}, \tag{30}$$

$$\phi_k=\frac{1}{2}\left(r_0+\mathrm{sgn}(k)\frac{a_-}{1+4\alpha}\right)$$
$$-a_-\mathrm{sgn}(k)\frac{1+\eta}{(1-\eta)^2}\eta^{|2k+1/2|+1/2}, \tag{31}$$

for any n, k. Note an identity

$$\eta^{|2k|}\pm\eta^{|2k+1|}\equiv 2|\eta|^{|2k+1/2|}g(\pm\eta,k),$$

$$g(\eta,k)=\begin{cases}\cosh(\frac{1}{2}\ln\eta), & \eta>0,\\ -\mathrm{sgn}(k)\sinh(\frac{1}{2}\ln|\eta|), & \eta<0,\end{cases}$$

which is valid for any k and $\eta\neq 0$. The appearance of Eqs. (30) and (31) suggests denoting $l_k=2k+\frac{1}{2}$. Using the identity $\mathrm{sgn}(l_k)\equiv\mathrm{sgn}(k)$, we obtain the following.

(a) For $\Sigma=\{--|++\}$:

$$\chi_k=u_0+l_k\rho^{(a)}(l_k)-2a_-\frac{\eta(1+\eta)[1-|\eta|^{|l_k|}g(\eta,l_k)]}{(1-\eta)^3},$$

$$\phi_k=\frac{1}{2}\rho^{(a)}(l_k)-a_-\mathrm{sgn}(l_k)\frac{(1+\eta)\,\eta^{|l_k|+1/2}}{(1-\eta)^2},$$

where $\rho(l_k)=w_{2k}$ for the infinite uniform chain of configuration $[\sigma_{2k}\sigma_{2k+1}]$: $\rho^{(a)}(l_k)=[r_0+\mathrm{sgn}(l_k)a_-(1+4\alpha)^{-1}]=r_s^{\pm}$, depending on the sign of l_k.

(b) For $\Sigma=\{+-|++\}$:

$$u_n=u_0+nr_s^+-2a_-\frac{\eta(1-\eta^n)}{(1-\eta)^3},\quad n\geqslant 0,$$

$$u_n=u_0+nr_0+a_-\zeta_n-2a_-\frac{\eta^2(1-\eta^{|n|})}{(1-\eta)^3},\quad n<0,$$

$$\chi_k=u_0+l_kr_s^+-2a_-\frac{\eta[1-|\eta|^{|l_k|}g(\eta,l_k)]}{(1-\eta)^3},\quad k\geqslant 0,$$

$$\chi_k=u_0+l_kr_0+\frac{1}{2}a_--2a_-\frac{\eta^2[1-|\eta|^{|l_k|}g(\eta,l_k)]}{(1-\eta)^3},\quad k<0,$$

$$\phi_k=\frac{1}{2}\rho^{(b)}(l_k)-\mathrm{sgn}(k)a_-\frac{\eta^{|2k|+1}}{(1-\eta)^2},$$

where $\zeta_n=[1-(-1)^n]/2$; $\rho^{(b)}(l_k)=r_s^+$ for $l_k>0$ and r_a^+ for $l_k<0$.

(c) For $\Sigma=\{-+|+-\}$:

$$u_n=u_0+nr_0+\mathrm{sgn}(n)2a_-\left[\zeta_n+2\frac{\eta(1-\eta^{|n|})}{(1-\eta)^2}\right],$$

$$\chi_k=u_0+l_kr_0+\mathrm{sgn}(l_k)2a_-\left[\frac{1}{2}+2\frac{\eta[1-|\eta|^{|l_k|}g(\eta,l_k)]}{(1-\eta)^2}\right],$$

$$\phi_k=\frac{1}{2}\rho^{(c)}(k)+\mathrm{sgn}(l_k)2a_-\frac{\eta|\eta|^{|l_k|}g(-\eta,l_k)}{(1-\eta)^2},$$

where $\rho^{(c)}(l_k)=r_a^{\pm}$, the sign in the superscript being that of l_k.

It is easy to see that the profiles of χ_k, ϕ_k have the solitonlike shape. In the next section we show that this similarity is not occasional, and that excitations of such a shape that behave as solitons can exist in the system.

D. Conditions of the existence and stability of static configurations of the chain

As was shown earlier [9,10], *every* local minimum of the system's potential energy (1) corresponds to a particular state $\{\sigma_n\}$ of the Ising model defined according to Eqs. (9)–(11). Meanwhile, the opposite is *not always* true. A sequence $\{\sigma_n\}$ corresponds to a local minimum of the system's potential energy, with interparticle distances $\{w_n\}$ given by Eq. (4) if only $C_1>0$ and

$$w_n>c \quad \text{for every } n \text{ such that } \sigma_n=+1, \tag{32}$$

$$0<w_n<c \quad \text{for every } n \text{ such that } \sigma_n=-1.$$

Sequences $\Sigma=\{\sigma_n\}$ obeying (not obeying) condition (32) will be referred to as *allowed* (*forbidden*) sequences. Let us find the conditions under which the configurations considered above are allowed.

It was shown in Ref. [10] that all possible configurations Σ are allowed if $a_1<a_2$, i.e., $a_->0$, inequality (8) holds, and all $w_n>0$. Let us divide both sides of Eq. (8) by $a_-(1-\eta)^2$ and express η through α in the left-hand side (lhs) of Eq. (8) with the help of Eq. (12). We easily obtain

$$|\tilde{c}-\tilde{r}_0|<\frac{(1+|\eta|)(1-3|\eta|)}{(1-\eta)^2}, \tag{33}$$

where

$$\tilde{r}_0=\frac{\tilde{a}+2\alpha\tilde{b}}{1+4\alpha}=\frac{r_0}{a_-},\quad \tilde{a}=\frac{a_+}{a_-},\quad \tilde{b}=\frac{b}{a_-},\quad \tilde{c}=\frac{c}{a_-}. \tag{34}$$

Parameter a_- plays here the role of a scale factor. It can be seen that the system's geometry may be exhaustively characterized (apart from the scale) by four dimensionless parameters $\{\tilde{a},\tilde{c},\tilde{r}_0,\alpha\}$.

Let us expand the modulus in the rhs of Eq. (33) and convert again η to α. Note also that, according to Eq. (12), $\eta>0$ implies $\alpha<0$, and vice versa. Moreover, the rhs of Eq. (33) must be positive in order for this inequality to hold. With this in mind, we find that *all* the configurations of the RSM are allowed if

$$\begin{aligned}|\tilde{c}-\tilde{r}_0|&<2\beta-\beta^2,\quad 1<\beta<2,\\ |\tilde{c}-\tilde{r}_0|&<2\beta-1,\quad 1/2<\beta<1,\end{aligned} \tag{35}$$

where $\beta=1/\sqrt{1+4\alpha}$. This result has a clear physical sense. The characteristic period of the chain r_0 has to be close enough to c, the location of the cusp in V_1, in order to enable two equilibrium lengths for every bond, one smaller and one greater than c. Otherwise only one of the branches of potential V_1 works, and this potential becomes effectively harmonic. In this case the solution of the equilibrium equation (3) is unique.

The condition that all w_n must be positive is to be satisfied simultaneously with Eq. (35). It is easy to see from Eq. (7) that

$$(w_n)_{\min}=r_0-y\frac{1+|\eta|}{1-|\eta|},$$

from which we obtain, with help of Eqs. (12), (13), and (34),

$$\tilde{r}_0>1,\quad \beta<1(\alpha>0), \tag{36}$$

$$\tilde{r}_0>\beta^2,\quad \beta>1(\alpha<0).$$

While all the states are allowed within the range of parameters given by the overlap of Eqs. (35) and (36), specific

TABLE I. Parameters Q_i from Eq.(37) for the simplest uniform and solitonlike configurations of the chain.

Σ	β	$q_1-\tilde{r}_0$	$q_2-\tilde{r}_0$	$q_3-\tilde{r}_0$
$\{++\}$	any β			β^2
$\{--\}$	any β	$-\beta^2$	$-\beta^2$	
$\{+-\}$	any β	-1	-1	1
$\{--\|++\}$	$\beta>1$	$-\beta^2$	$-\beta$	β
	$\beta<1$	$-\beta$	$-\dfrac{\beta(3\beta-1)}{\beta+1}$	$\dfrac{\beta(3\beta-1)}{\beta+1}$
$\{+-\|++\}$	$\beta>1$	-1	$\frac{1}{2}(\beta-1)^2-1$	1
	$\beta<1$	-1	$\frac{1}{2}(\beta-1)^2-1$	$\frac{1}{2}(\beta+1)^2-1$
$\{-+\|+-\}$	$\beta>1$	-1	$\dfrac{(\beta-1)^2}{\beta+1}-1$	1
	$\beta<1$	-1	$\dfrac{(\beta-1)^2}{\beta+1}-1$	β

configurations may exist in a wider range of parameters. In order to find this range for a particular configuration Σ, we have to estimate three values,

$$Q_1(\Sigma)=a_-^{-1}\min_{\Sigma} w_n \quad \text{for such } n \text{ that } \sigma_n=-1,$$

$$Q_2(\Sigma)=a_-^{-1}\max_{\Sigma} w_n \quad \text{for such } n \text{ that } \sigma_n=-1, \tag{37}$$

$$Q_3(\Sigma)=a_-^{-1}\min_{\Sigma} w_n \quad \text{for such } n \text{ that } \sigma_n=+1,$$

and to find conditions under which $0<Q_1$, $Q_2<\tilde{c}<Q_3$. Note that $Q_1\leqslant Q_2$ by definition (37). Parameters Q_i for the configurations Σ considered above may be calculated using Eqs. (7), (21), and (26). They are summarized in Table I.

III. ANALYTICAL DESCRIPTION OF SOLITONIC TRANSFORMATIONS OF THE RSM

While the static RSM can be solved exactly and analytically, the dynamic version of the model does not allow an exhaustive analytical treatment. The dynamic properties of the RSM and its modifications have been investigated with the help of numerical and analytical methods [13–17].

On the basis of this research, Schilling *et al.* argued that, for low enough temperatures and small $|\eta|$, the dynamics is reduced to the vibrations in the vicinity of particular local minima and transitions between them. Moreover, the overwhelming kind of process $\{\sigma_j\}\to\{\sigma_j'\}$, where $\sigma_j=\sigma(w_j(t))$, $\sigma_j'=\sigma(w_j(t+\Delta t))$, has been found to be single spin flips, i.e., transitions (sudden changes of w_j) that $\sigma_j'=-\sigma_j$, but $\sigma_k'=\sigma_k$ for all $j\neq k$. Hence, under these conditions the localized processes play the predominant role in RSM dynamics.

However, at a quench from high to low temperature the system generally cannot reach its ground state. Since the potential landscape is very complex and every two neighboring local minima are separated by a barrier, the global minimum (the ground state) of the infinite system cannot be reached within finite time. As a result of relaxation, the system becomes frozen in a metastable state, the excessive free energy of which is determined by the quench rate. Analysis of the relaxation process shows that, at finite times, localized transformations may only lead to formation of a block-copolymer-like state, which is still metastable. Further transformation into a uniform ground state may be only brought about by movement and annihilation of block boundaries, or topological defects. Therefore, it may be argued that solitonic transformations are dominating at late stages of the quench of initially disordered systems.

Moreover, while $|\eta|$ increases from 1/3 to 1, which corresponds to $\alpha\to-1/4$ or $\alpha\to+\infty$, the correlation length in the allowed states increases infinitely. Therefore, most single-spin flips would lead from allowed to forbidden states. In this case the cooperative dynamic processes may play a major role and influence significantly the kinetic and thermal properties of a RSM-like system.

A. Exact discrete equations of motion

The system's Hamiltonian is obtained from Eq. (1) by addition of the kinetic energy term,

$$\mathcal{H}=\frac{1}{2}\sum_n [m\dot{u}_n^2+V_1(u_{n+1}-u_n)+V_2(u_{n+2}-u_n)].$$

In terms of the molecular variables χ_k, ϕ_k introduced in Eq. (29) the Hamiltonian takes the form

$$\mathcal{H}=\sum_k [m(\dot{\chi}_k^2+\dot{\phi}_k^2)+V_1(2\phi_k)+V_1(\chi_k-\phi_k-\chi_{k-1}-\phi_{k-1})+V_2(\chi_k-\phi_k-\chi_{k-1}+\phi_{k-1})+V_2(\chi_k+\phi_k-\chi_{k-1}-\phi_{k-1})].$$

Let us rewrite Eq. (2) for the NN potential to separate the parabolic part and the piecewise-linear term $U(x)$ that brings about the nonlinearity of the system,

$$V_1(x)=\frac{1}{2}C_1[(x-a_1)^2-(c-a_1)^2]+C_1U(x),$$

$$U(x)=-2a_-(x-c)\theta(x-c),$$

where $\theta(x)=[\mathrm{sgn}(x)+1]/2$ is the step function. Then the equations of motion are as follows:

$$2m\frac{d^2\chi_k}{dt^2}-(C_1+2C_2)(\chi_{k+1}-2\chi_k+\chi_{k-1})+C_1(\phi_{k+1}-\phi_{k-1})-C_1U'(\delta_{k+1})+C_1U'(\delta_k)=0, \tag{38}$$

$$2m\frac{d^2\phi_k}{dt^2}-C_1(\chi_{k+1}-\chi_{k-1})+8C_1\phi_k+(C_1-2C_2)(\phi_{k+1}-2\phi_k+\phi_{k-1})-C_1U'(\delta_{k+1})-C_1U'(\delta_k)+2C_1U'(2\phi_k)=0, \tag{39}$$

where $\delta_k=(\chi_k-\phi_k-\chi_{k-1}-\phi_{k-1})=w_{2k-1}$ are distances between neighboring "atoms" of different "molecules."

In general, both series of equations (38) and (39) are nonlinear since $U(x)$ has a cusp at point $x=c$. However, $U'(\delta_k)=-2a_-\theta(\delta_k-c)=\mathrm{const}$ for a special class of solutions. Consider a process where all the intermolecular bonds, both before and after the transformation, are either compressed ($\delta_k<c$) or stretched ($\delta_k>c$). Then $U'(\delta_{k+1})-U'(\delta_k)\equiv 0$, and Eq. (38) becomes linear.

Let us suppose, moreover, that all the intramolecular bonds have the same "sign" before the transformation (at $t\to-\infty$ for every fixed k) and change it to the opposite sign after transformation (at $t\to+\infty$ for given k). Then Eq. (39) becomes linear in each of these limits. Thus, we restrict the consideration by one particular (but very important) class of process, $\Sigma\to\Sigma'$, where $\Sigma=\{\sigma_1\sigma_2\}$, $\Sigma'=\{\sigma_1'\sigma_2\}$, where $\sigma_1'=-\sigma_1$.

B. Continualized equations of motion

Since discrete equations (38) and (39), even upon the above simplification, are still intractable, let us continualize them. We will look for smooth running-wave-type solutions. One of the configurations Σ and Σ' is always an AUS. In the AUS the distance between the centers of neighboring molecules $\chi_{k+1}-\chi_k=r_a^++r_a^-=2r_0$, therefore, it seems natural to introduce the wave variable ξ according to

$$\chi_k(t)\equiv\chi(\xi),\quad \phi_k(t)\equiv\phi(\xi),\quad \xi=2kr_0-vt,$$

where v is the wave velocity. As shown above, Eqs. (38) and (39) are linear in the limit $\xi\to\pm\infty$. We take account of the fact that $U'(2\phi)=-a_-(\mathrm{sgn}(\phi-c/2)+1)$, $U'(\delta_k)\equiv -a_-(\sigma_2+1)$. After developing the finite differences in Eqs. (38) and (39) into series over r_0 as a small parameter, we obtain in the leading orders:

$$4s^2r_0^2\chi''-4(1+2\alpha)\left(r_0^2\chi''+\frac{1}{3}r_0^4\chi^{(IV)}+\frac{2}{45}r_0^6\chi^{(VI)}+\cdots\right)+4\left(r_0\phi'+\frac{2}{3}r_0^3\phi'''+\frac{2}{15}r_0^5\phi^{(V)}+\cdots\right)=0, \tag{40}$$

$$4s^2r_0^2\phi''-4\left(r_0\chi'+\frac{2}{3}r_0^3\chi'''+\frac{2}{15}r_0^5\chi^{(V)}+\cdots\right)+4(1-2\alpha)\times\left(r_0^2\phi''+\frac{1}{3}r_0^4\phi^{(IV)}+\cdots\right)+8\phi+2a_-\times[\sigma_2-\mathrm{sgn}(\phi-c/2)]=0, \tag{41}$$

where $s=(v/r_0)\sqrt{m/2C_1}$ is the dimensionless velocity and the prime denotes $d/d\xi$. Let us note that in general $\phi=O(1)$, $\chi'=O(1)$. Since Eq. (40) is linear, we can represent χ in the form of a series,

$$\chi'=G+g_0\phi+\sum_{i=1}^{\infty}g_i\phi^{(i)}. \tag{42}$$

Finding the constants G and g_i will solve our problem. Let us substitute Eq. (42) into Eq. (40) and note that at $\phi\not\equiv 0$ the coefficients at every derivative of ϕ must vanish independently. Thus, the coefficient at ϕ' is equal to

$$4r_0^2g_0[s^2-(1+2\alpha)]+4r_0=0;$$

therefore, $g_0=(r_0p)^{-1}$, where $p=1+2\alpha-s^2$. By analogy, we obtain

$$g_1=g_3=g_5=\cdots=0,\quad g_2=\frac{r_0}{3p^2}(2p-p_0),$$

$$g_4=\frac{r_0^3}{45p^3}(6p^2-12p_0p+5p_0^2),\ \ldots, \tag{43}$$

where we denoted $p_0=1+2\alpha$. Below we cut the series expansion (42) on the fourth term. Let us substitute Eq. (42) with coefficients from Eq. (43) (only G is still unknown) into Eq. (41). This yields

$$B_0\phi+B_2\phi''+B_4\phi^{(IV)}+\cdots=r_0G+\frac{1}{2}a_-[\mathrm{sgn}(\phi-c/2)-\sigma_2], \tag{44}$$

$$B_0=2-p^{-1},\quad B_2=-\frac{r_0^2}{p}\left((p-1)^2+\frac{p-p_0}{3p}\right),$$

$$B_4=-\frac{r_0^4}{3p}\left\{(p-1)^2+(p-p_0)\left[-p+\frac{17p-5p_0}{15p^2}\right]\right\}. \tag{45}$$

To establish the boundary conditions let us note that the configuration of the part of the chain not yet affected by the transformation ($\xi\to+\infty$) is merely a certain static configuration, $\Sigma=\{\sigma_1\sigma_2\}$. Taking into account Eqs. (20), (24), and (29), we find that

$$\phi|_{\xi\to+\infty}=\frac{1}{2}r(\{\sigma_1\sigma_2\})$$
$$=\frac{1}{2}\left\{c+\frac{a_-}{1+4\alpha}[\sigma_1+2\alpha(\sigma_1-\sigma_2-\psi)]\right\},$$
$$\phi'|_{\xi\to+\infty}=\phi''|_{\xi\to+\infty}=\cdots=0. \qquad (46)$$

Moreover, ϕ must be bounded for $\xi\to-\infty$.

Equation (44) with boundary conditions (46) has been solved in the Appendix. The correspondence between problems (44),(46) and (A5),(A6) is as follows:

$$y=\phi-\frac{c}{2},$$

$$y_0=\frac{r(\{\sigma_1\sigma_2\})-c}{2}=\frac{a_-[\sigma_1+2\alpha(\sigma_1-\sigma_2-\psi)]}{2(1+4\alpha)}, \qquad (47)$$

$$A_1=-\frac{a_-}{2},\quad A_2=-r_0G+\frac{B_0c+a_-\sigma_2}{2}. \qquad (48)$$

Note that $\mathrm{sgn}(y_0)=\sigma_1$. Then the necessary condition of existence of a solution for the problem involved is given by Eq. (A8),

$$y_0=[r_0G+a_-(\sigma_1-\sigma_2)/2]/B_0-c/2. \qquad (49)$$

Comparison of Eqs. (48) and (49) yields

$$A_2=-B_0y_0+\sigma_1a_-/2.$$

C. Sound velocity

The sound velocity is determined by periodic solutions of Eq. (44) that have infinitely small spatial frequency $\Omega=i\lambda_1$, where λ_1 is given by Eq. (A2) or, in the limit $|q_2|\ll1$, by Eq. (A4). In the latter case, upon substitution of the values of coefficients B_i from Eq. (45), the condition $\Omega=0$ reads as $B_0/B_2=0$. Since $B_0=0$ for $p=1/2$, we only have to ensure that $B_2\neq0$ and $|q_2|\ll1$ for $p=1/2$. If $p=1+2\alpha-s^2=1/2$, then $p-p_0=-s^2=-(1+4\alpha)/2$ and

$$B_2=2r_0^2\left(\frac{1+4\alpha}{3}-\frac{1}{4}\right)=\frac{r_0^2}{6}(1+16\alpha)=0,$$

if only $\alpha=-1/16$, which is outside the range allowed for α. Furthermore, for $p=1/2$,

$$B_4=-\frac{2r_0^4}{3}\left\{\frac{1}{4}-\frac{1+4\alpha}{2}\left[-\frac{1}{2}+\frac{4}{15}\left(6-\frac{5}{2}(1+4\alpha)\right)\right]\right\}$$
$$=-\frac{4r_0^4}{45}(7+33\alpha+80\alpha^2)<0.$$

As shown in the Appendix, two kinds of solutions may exist, the first one corresponding to a topological soliton (kink). An additional condition of its existence is given by Eq. (A37), which allows one to find G using Eq. (48):

$$G=\frac{B_0c+a_-\sigma_2}{2r_0}=\frac{(2-p^{-1})\tilde{c}+\sigma_2}{2\tilde{r}_0}.$$

Now $y_0=-\sigma_1A_1/B_0$. Let us substitute y_0 from Eq. (47), A_1 from Eq. (48), and B_0 from Eq. (44), then

$$\frac{\sigma_1a_-}{2(2-p^{-1})}=\frac{a_-[\sigma_1+2\alpha(\sigma_1-\sigma_2-\psi)]}{2(1+4\alpha)}.$$

Let us remember that $p=1+2\alpha-s^2$. After simple transformations we obtain the unique value of the kink velocity,

$$p=\frac{1}{2}\left(1+\frac{1+4\alpha}{1+\epsilon}\right),\quad s_K=\left[\frac{(1+4\alpha)\epsilon}{1+\epsilon}\right]^{1/2}, \qquad (50)$$

where

$$\epsilon=-4\alpha\sigma_1(\sigma_2+\psi). \qquad (51)$$

Since $\alpha>-1/4$, kink propagation is only possible if $\epsilon\geqslant0$. In particular, $\epsilon=0$ corresponds to the stationary kink.

It is easy to see from Eq. (44) that the velocity spectrum of nontopological solitons (NTSs) is bounded from below by the kink velocity s_K while the upper limit for the NTS velocity, $s_{\max}$, is given by conditions $B_0>0$, $B_2<0$ [see Eq. (45)]. Therefore, $0<s_K<s_{\mathrm{NTS}}<s_{\max}$, where

$$s_{\max}^2=\begin{cases}1, & -\frac{1}{4}<\alpha<-\frac{1}{16},\\ \dfrac{1+6\alpha-\sqrt[3]{1+18\alpha}}{\frac{3}{2}(1+4\alpha)}, & \alpha\geqslant-\frac{1}{16}.\end{cases}$$

Note that $s_{\max}\simeq|\alpha|2\sqrt{6}$ for for $|\alpha|\ll1$.

D. Kink energy and profile

The kink profile is given by Eq. (A38) taking into account Eq. (47),

$$\phi(\xi)=\frac{c}{2}+\mathrm{sgn}(\xi)\frac{r-c}{2}[\Lambda_1(1-e^{-\lambda_1|\xi|})+\Lambda_2(1-e^{-\lambda_2|\xi|})], \qquad (52)$$

where $r=r(\{\sigma_1\sigma_2\})$ is given by Eq. (24) and parameters λ_i, Λ_i may be calculated with the help of Eqs. (A2), (A19), (A20), (45) and (50). It is easy to see without calculation that, while $\phi(+\infty)=r/2$, in the opposite limit $\phi(-\infty)=c-r/2$.

A running soliton transfers the chain from an initial equilibrium state to a dynamic intermediate one. The intermediate state then relaxes to the a new equilibrium one. The former differs from the latter by the fact that all particles have nonzero velocities.

The energy of the final static configuration E_f, the initial static configuration E_i, and the intermediate dynamic configuration E_d can be found by substitution of interatomic distances calculated according to Eq. (52) into Eq. (15). This yields $E_f-E_i=e_0\epsilon^2$ for static states, where ϵ is given by Eq. (51). This means that, if the kink is possible (i.e., $\epsilon>0$), then its propagation is an endothermic process because $e_0>0$. The kinetic energy of particles in the intermediate dynamic state turns out to be exactly equal to the relative potential energy (E_d-E_i). Thus, the Lagrangians of the initial and intermediate states coincide. Therefore, in this case the Lagrangian is conserved upon transformation and thus plays the role of "effective energy."

While continualizing the discrete equations of motion (38) and (39) we have neglected ϕ''' and higher-order derivatives. It is only justified if ϕ changes slightly on the scale of several lattice constants. In other words, the continuous theory is valid if the width ξ_0 of the soliton front is much larger than r_0. Kink front width may be found from Eq. (45),

$$\xi_0=\sqrt{-B_2/B_0}$$
$$=r_0(2p-1)^{-1/2}\left[(p-1)^2+\frac{1}{3}\left(1-\frac{1+2\alpha}{p}\right)\right]^{1/2}.$$

In particular, for a stationary kink $(s_K=0)$,

$$\xi_0=r_0\frac{2|\alpha|}{\sqrt{1+4\alpha}}. \tag{53}$$

This result is to be compared to the front width ξ_{RS} given by exact discrete Reichert-Schilling theory. The latter yields, as suggested by Eqs. (4) and (5),

$$\xi_{\mathrm{RS}}=r_0|\ln|\eta||^{-1}=r_0\left|\ln\left|\frac{-1-2\alpha+\sqrt{1+4\alpha}}{2\alpha}\right|\right|^{-1}. \tag{54}$$

To compare Eqs. (53) and (54) let us consider two asymptotic cases.

(a) $\mu_1\equiv(1+4\alpha)\to 0$:

$$\xi_0\simeq\tfrac{1}{2}r_0\mu_1^{-1/2}(1-\mu_1),\qquad \xi_{\mathrm{RS}}\simeq\tfrac{1}{2}r_0\mu_1^{-1/2}(1+\mu_1);$$

(b) $\mu_2\equiv\alpha^{-1}\to 0$:

$$\xi_0\simeq\tfrac{1}{2}r_0\mu_2^{-1/2}(1-\tfrac{1}{8}\mu_2),\qquad \xi_{\mathrm{RS}}\simeq\tfrac{1}{2}r_0\mu_2^{-1/2}(1+\tfrac{3}{8}\mu_2).$$

Thus, the prediction of the approximate continuous theory coincides in the leading order with the exact result for the static case. This encourages application of the above continualization approach to the investigation of the dynamic Reichert-Schilling model and structural transformations in more general nondegenerate systems.

IV. SOLITONIC TRANSFORMATIONS IN A SMOOTH-POTENTIAL RSM-LIKE MODEL: NUMERICAL APPROACH

As shown in the previous section, topological solitons may exist in the RSM under certain conditions. These solitons, however, turn out to be unstable due to the presence of a cusp in the NN potential. Our idea is to consider more realistic RSM-type models using a smoothening procedure.

The potentials of interaction in real molecular and atomic chains are smooth functions of displacement. Besides, nonsmoothness leads to instability of the numerical procedures of integration. Therefore, let us start by smoothening the NN potential. Consider the potential given by the following expression:

$$V_{1,\delta}(x)=\frac{1}{2}C_1(x-a_1)^2+U_\delta(x), \tag{55}$$

where the function $U_\delta(x)$ is the smooth version of $U_0(x)$,

$$U_\delta(x)=\frac{1}{2}k(x-c)-\sqrt{\delta^2+\frac{1}{4}k^2(x-c)^2},\quad k=-2C_1a_-, \tag{56}$$

δ is the smoothening parameter, and only the positive value of the square root is considered. At $\delta\neq 0$, the functions (55) and (56) depend smoothly on u. At $x\to\infty$, the potential (55) tends asymptotically to $V_1(x)$, and at $\delta\to 0$ the function $V_{1,\delta}(x)$ tends uniformly to $V_1(x)$.

The piecewise-parabolic potential is a two-well potential at $a_1<c<a_2$ and one-well at $c\leqslant a_1$ or $a_2\leqslant c$. At $c=(a_1+a_2)/2$, function (56) becomes a symmetrical two-well potential; therefore, the smoothened potential (55) has a symmetrical two-well shape [Fig. 1(a)]. Characteristic profiles of the interaction potentials at $c>a_2$ are drawn in Fig. 1(b).

A. Uniform stationary states

To find the interparticle distances for a stationary uniform state of the chain with smoothened NN potential $V_{1,\delta}$ one should minimize numerically the corresponding energy:

$$\mathcal{E}_{\mathrm{st},\delta}=V_{1,\delta}(x)+V_2(2x)\to\min_x, \tag{57}$$

for the simple uniform states and

$$\mathcal{E}_{\mathrm{st},\delta}=\frac{1}{2}[V_{1,\delta}(x_1)+V_{1,\delta}(x_2)]+V_2(x_1+x_2)\to\min_{x_1,x_2}, \tag{58}$$

for alternating uniform states. These problems were solved by the method of steepest descent. Equation (57) has two solutions, $r^{\pm}_{s,\delta}$, while Eq. (58) has one solution, $(r^-_{a,\delta},r^+_{a,\delta})$. Substitution of these solutions into expressions (57) and (58) yields the energies of the stationary states $\mathcal{E}^{\{--\}}_{\mathrm{st},\delta}$, $\mathcal{E}^{\{++\}}_{\mathrm{st},\delta}$, and $\mathcal{E}^{\{+-\}}_{\mathrm{st},\delta}\equiv\mathcal{E}^{\{-+\}}_{\mathrm{st},\delta}$. The uniform states $\{--\}$, $\{-+\}$, and $\{+-\}$ of the chain are schematically represented by Fig. 2.

A natural analogy of the system in question and a polymer chain appears. The system in the alternating uniform state may be considered as a chain of repeating segments (mono-

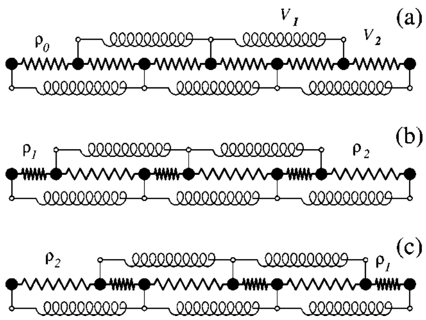

FIG. 2. Schematic representation of (a) the uniform stationary state of the chain $\{--\}$ ($x=r^-_{s,\delta}$), (b) the alternating uniform states $\{-+\}$, and (c) $\{+-\}$ ($x_1=r^-_{a,\delta}$, $x_2=r^+_{a,\delta}$).

mers), each of them consisting of two bonds of different length, one compressed $(-)$ and one stretched $(+)$. Since the transition $(-)\leftrightarrow(+)$ is reversible, such states may be considered as different conformational states, e.g., *cis* and *trans*. Uniform state $\{--\}$ is the intermediate point of a transition between them.

To describe the "conformational" transformation $\{-+\}\to\{+-\}$, new coordinates can be introduced:

$$r=u_1,\quad w=u_1+u_2-l,\quad \text{where}\quad l=r^+_{a,\delta}+r^-_{a,\delta} \tag{59}$$

is the monomer length for the system in the alternating stationary state. Here r describes the "conformational" state of the monomer, and w is the change of the "molecular chain" step. Potential surface of the conformational transition is given by the following expression:

$$E(r,w)=\frac{1}{2}[V_{1,\delta}(r)+V_{1,\delta}(l+w-r)]+V_2(l+w).$$

Consider, for example, two sets of chain parameters,

$$a_1=1,\ a_2=3,\ c=2,\ b=4.5,\ \alpha=1,\ \delta=0.4, \tag{60}$$

$$a_1=1,\ a_2=3,\ c=3.5,\ b=6.5,\ \alpha=1,\ \delta=0.4, \tag{61}$$

with $C_1=1$, $C_2=\alpha$. For the set (60) the NN potential is a symmetrical double-well potential [see Fig. 1(a)]. At any value of the parameter $\alpha>0$ the ground state is $\{-+\}$. The dependence of the values $r^-_{s,\delta}$, $r^\pm_{a,\delta}$, $\mathcal{E}^{\{--\}}_{\mathrm{st},\delta}$, and $\mathcal{E}^{\{-+\}}_{\mathrm{st},\delta}$ on α is demonstrated in Table II.

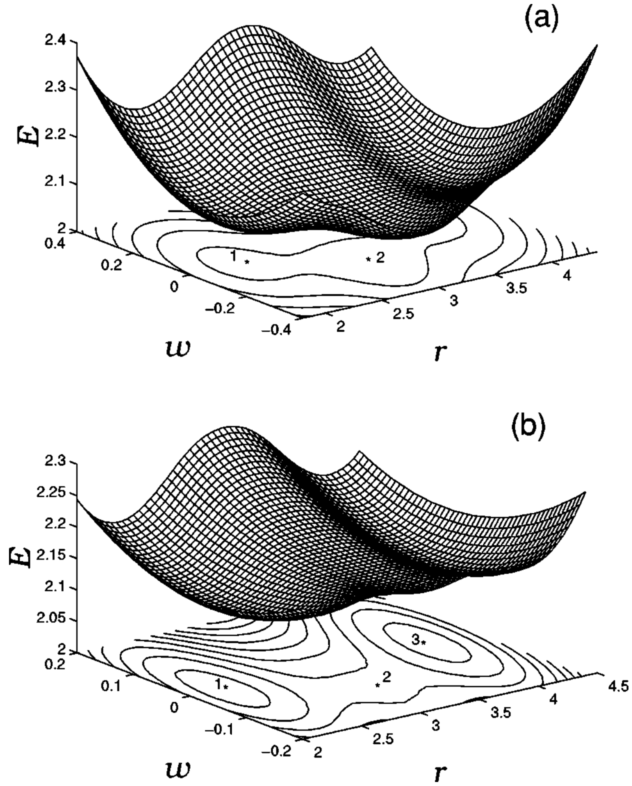

FIG. 3. Potential surface $E(r,w)$ of the conformational transformation $\{-+\}\to\{+-\}$ for (a) $a_1=1$, $a_2=3$, $b=6.5$, $\alpha=1.7$, $\alpha=1$, $\delta=$ 0.4 [point 1 corresponds to the state $\{-+\}$ ($r=2.2409$, $w=0$, $E_{\{-+\}}=2.1811$), point 2 is for $\{--\}$ ($r=2.9888$, $w=-0.1713$, $E_{\{--\}}=2.0717$)]; and for (b) $a_1=1$, $a_2=3$, $b=6.5$, $\alpha=3$, $\alpha=1$, $\delta=0.4$ [point 1 corresponds to the state $\{-+\}$ ($r=2.2765$, $w=0$, $E_{\{-+\}}=2.1297$), point 2 is for $\{--\}$ ($r=3.0994$, $w=-0.0967$, $E_{\{--\}}=2.1743$)].

For the set of values (61) the NN interaction potential is the single-well type [see Fig. 1(b)]. The ground state is $\{--\}$ for $\alpha<\alpha_0\approx1.8668$, or $\{-+\}$ for $\alpha>\alpha_0$. Let us consider the potential surface of the structural transition $E(r,w)$ (Fig. 3). At $\alpha<\alpha_0$ the conformational transition $\{-+\}\to\{+-\}$ is impossible because the state $\{--\}$, which is the intermediate point of the transition, has lower energy than the final state $\{+-\}$ [see Fig. 3(a)]. Therefore, the system would be "caught" in the state $\{--\}$. At $\alpha\geqslant\alpha_0$ this cannot take place because now the state $\{--\}$ has higher energy than $\{-+\}$ and $\{+-\}$ [see Fig. 3(b)]. In this case the exis-

TABLE II. Dependence of the values $r^-_{s,\delta}$, $r^\pm_{a,\delta}$, $\mathcal{E}^{\{--\}}_{\mathrm{st},\delta}$, and $\mathcal{E}^{\{-+\}}_{\mathrm{st},\delta}$ on α for model parameters (60).

α	$r^-_{s,\delta}$	$r^-_{a,\delta}$	$r^+_{a,\delta}$	$\mathcal{E}^{\{--\}}_{\mathrm{st},\delta}$	$\mathcal{E}^{\{-+\}}_{\mathrm{st},\delta}$
0.1	1.3571	1.1660	2.9956	0.0970	−0.0715
1.0	2.0000	1.3033	3.1114	0.0487	−0.0585
2.0	2.1111	1.3255	3.1281	0.0544	−0.0565
5.0	2.1905	1.3410	3.1394	0.0575	−0.0551
10.0	2.2195	1.3466	3.1434	0.0586	−0.0547
25.0	2.2376	1.3501	3.1459	0.0592	−0.0544
50.0	2.2438	1.3513	3.1467	0.0594	−0.0543

TABLE III. Dependence of the values $r^-_{s,\delta}$, $r^{\pm}_{a,\delta}$, $\mathcal{E}^{\{--\}}_{\mathrm{st},\delta}$, and $\mathcal{E}^{\{-+\}}_{\mathrm{st},\delta}$ on α for model parameters (61).

α	$r^-_{s,\delta}$	$r^-_{a,\delta}$	$r^+_{a,\delta}$	$\mathcal{E}^{\{--\}}_{\mathrm{st},\delta}$	$\mathcal{E}^{\{-+\}}_{\mathrm{st},\delta}$
1.8668	2.9843	2.2458	3.9332	2.09256	2.09256
2.0	3.0000	2.2500	3.9494	2.10682	2.09899
5.0	3.1429	2.3037	4.0711	2.22882	2.15529
10.0	3.1951	2.3269	4.1094	2.26950	2.17521
25.0	3.2277	2.3420	4.1323	2.29363	2.18750
50.0	3.2388	2.3472	4.1399	2.30161	2.19166

tence of a stable stationary state $\{--\}$ is not an obstacle for the conformational transition $\{-+\}\rightarrow\{+-\}$. The dependence of the bond lengths and energies on α for a system with parameters (61) is given in Table III.

B. Topological defects of the alternating uniform state

Let us consider now topological solitons that bring about the transition between two alternating states with equal energies, $\{-+\}$ and $\{+-\}$. We will call the defect in the chain $\{-+|+-\}$ *positive* and in the chain $\{+-|-+\}$ *negative*. Below we show that these defects possess solitonic features, i.e., they are actually topological solitons of different signs.

Consider a chain of $2N+1$ particles, u_n being the coordinate of the nth particle, $n=0,1,\dots,2N$. For the stationary state $\{-+\}$ $w_{2k}=r^-_{a,\delta}$, $w_{2k+1}=r^+_{a,\delta}$, and for the state $\{+-\}$ $w_{2k}=r^+_{a,\delta}$, $w_{2k+1}=r^-_{a,\delta}$, $n=0,1,\dots,N-1$. To find the stationary topological defect the minimization problem must be solved:

$$\mathcal{P}=\sum_{k=1}^{N-2}\left[V_{1,\delta}(w_{2k})+V_{1,\delta}(w_{2k+1})+V_2(w_{2k}+w_{2k+1})\right]+\sum_{k=1}^{N-1}\left[V_2(w_{2k-1}+w_{2k})\right]\rightarrow\min_{w_{2k},w_{2k+1}},\quad 1\leqslant k\leqslant N-2, \tag{62}$$

with boundary conditions

$$w_0=r^-_{a,\delta},\quad w_1=r^+_{a,\delta},\quad w_{2N-2}=r^+_{a,\delta},\quad w_{2N-1}=r^-_{a,\delta}, \tag{63}$$

for positive defect, and

$$w_0=r^+_{a,\delta},\quad w_1=r^-_{a,\delta},\quad w_{2N-2}=r^-_{a,\delta},\quad w_{2N-1}=r^+_{a,\delta}, \tag{64}$$

for negative defect.

The following defect parameters may be defined: the defect center position,

$$P=\sum_{k=0}^{N-2}k(w_{2n+2}-w_{2n})/S,$$

$$S=\sum_{k=0}^{N-2}(w_{2n+2}-w_{2n})=w_{2N-2}-w_0, \tag{65}$$

the defect radius,

$$R=\left\{\sum_{k=0}^{N-2}(p-k)^2(w_{2n+2}-w_{2n})/S\right\}^{1/2}, \tag{66}$$

and diameter, $L=2R+1$. All the values P, R, and L are dimensionless as they are expressed in the chain units. It is convenient to introduce a new variable, the change in the period of the molecular chain $z_n=w_{2n}+w_{2n+1}-(r^+_{a,\delta}+r^-_{a,\delta})$. Then the soliton amplitude may be defined as $A=z_{k_0}$, where k_0 is determined by the condition $|z_{k_0}|=\max_k|z_k|$. For a positive defect w_{2k} varies monotonically from $r^-_{a,\delta}$ to $r^+_{a,\delta}$, and for a negative defect vice versa (Fig. 4).

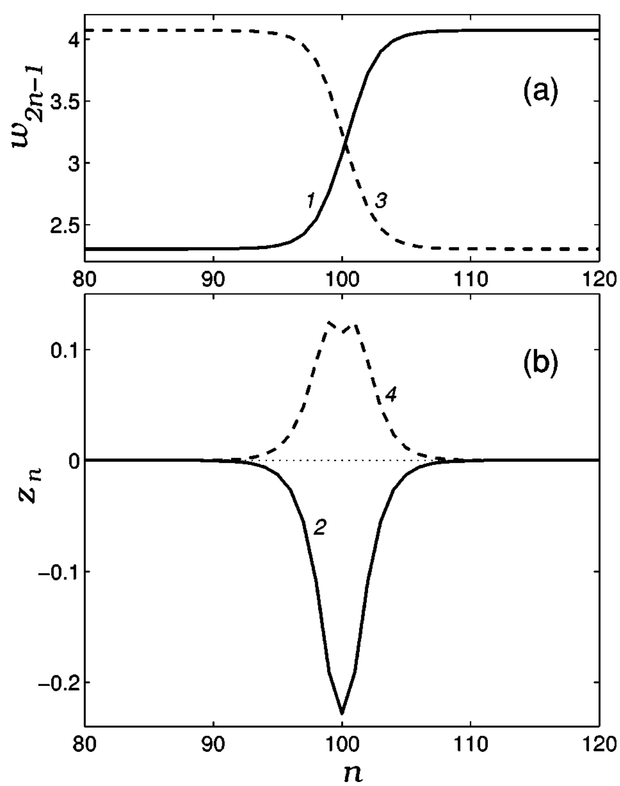

FIG. 4. Positive (curves 1, 2) and negative (curves 3, 4) stationary defects of the chain at $a_1=1$, $a_2=3$, $b=6.5$, $c=3.5$, $\alpha=5$, $\delta=0.4$. The defect parameters are $L_+=5.546$, $A_+=-0.2282$; $L_-=5.529$, $A_-=0.1242$. The energy of the pair formation $\Delta E=2.1026$.

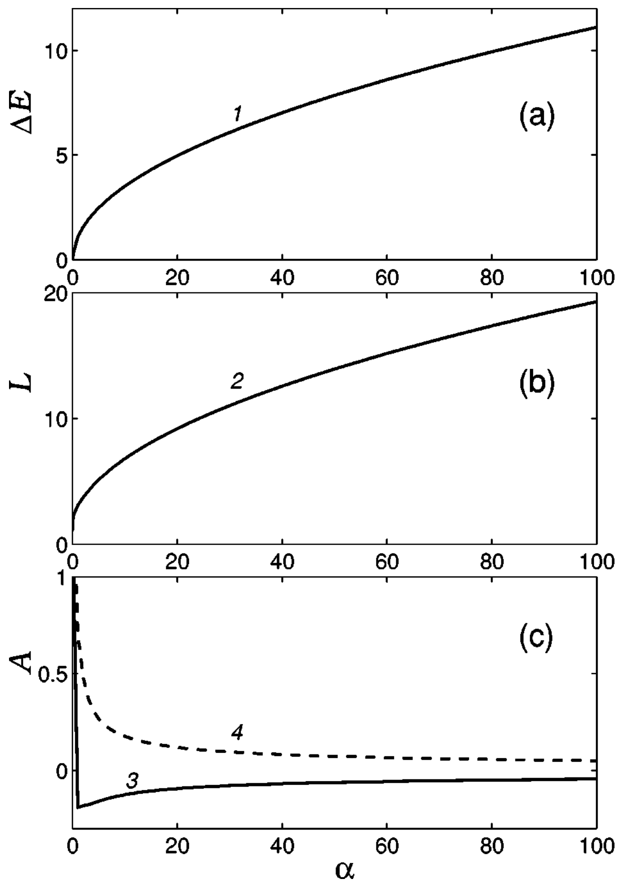

FIG. 5. The dependence of the formation energy of the defect pair, ΔE (curve 1), diameters $L_{\pm}$, and amplitudes $A_{\pm}$ (curves 3, 4) on α for $a_1=1,\ a_2=3,\ b=4.5,\ c=2,\ \delta=\ 0.4$.

Let us define also the defect energy $E=\mathcal{P}-\mathcal{P}_0$, where $\mathcal{P}$ is given by Eq. (62) and $\mathcal{P}_0$ is the energy of the defect-free chain,

$$\mathcal{P}_0=N[V_{1,\delta}(r^+_{a,\delta})+V_{1,\delta}(r^-_{a,\delta})]+(2N-1)V_2(r^+_{a,\delta}+r^-_{a,\delta}).$$

Let us note that only the energy of a pair of defects of different sign, $\Delta E=E_++E_-$, has a physical sense, since the defects may only be formed in pairs from an initially homogeneous state.

A typical appearance of stationary defects is shown in Fig. 4. The defects have the kink-shaped profile characteristics of topological solitons. In the region of soliton localization, local chain compression takes place for positive defects and stretching takes place for negative defects. A topological defect (soliton) describes the subsequent transformation of the chain from one AUS to another. In the defect center the chain is in the nonalternating uniform state. Such a defect may be stable if only the alternating state has lower energy than the nonalternating one. Otherwise the whole chain would transfer from two AUS's to the corresponding SUS. Therefore, for the set of parameters (60) the defects are stable for any α, and for Eq. (61) only for $\alpha\geqslant 1.8668$. The dependence of the defect pair energy ΔE, diameter $L_{\pm}$, and amplitude $A_{\pm}$ on α for these sets of parameters is shown in Figs. 5 and 6.

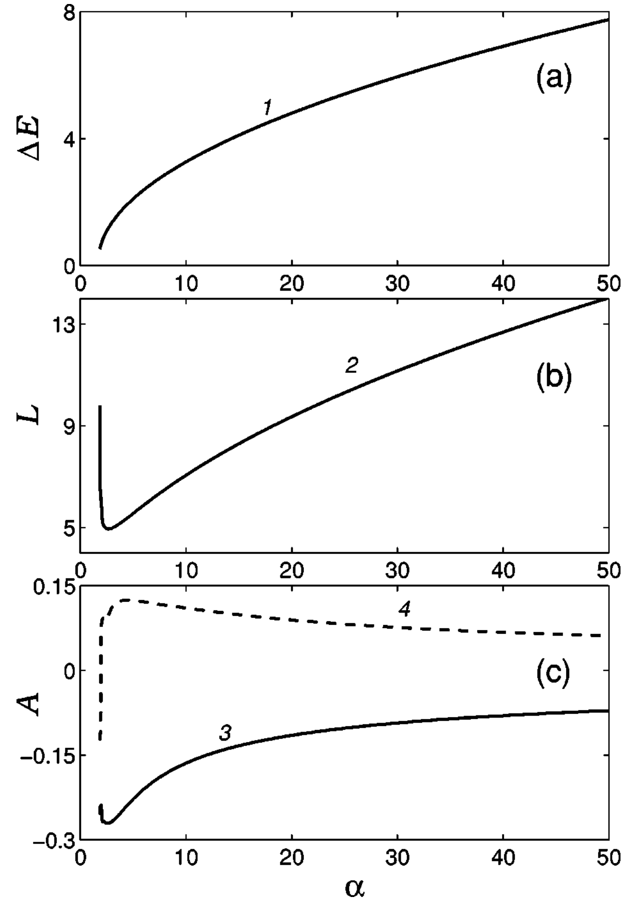

FIG. 6. The dependence of the formation energy of the defect pair ΔE (curve 1), diameters $L_{\pm}$, and amplitudes $A_{\pm}$ (curves 3, 4) on α for $a_1=1,\ a_2=3,\ b=6.5,\ c=3.5,\ \delta=\ 0.4$.

C. Dynamics of topological defects

Suppose that a topological defect moves as a constant-profile wave, then [see Eqs. (29) and (59) for definitions of the variables involved]

$$\chi_n=\chi(nl-vt),\quad \phi_n=\phi(nl-vt),$$

where v is the defect velocity, and $\chi(\xi),\ \phi(\xi)$ are smooth functions of the wave variable $\xi=nl-vt$. Let us replace the time derivatives $\dot{\chi}_n,\ \dot{\phi}_n$ by increments,

$$\dot{\chi}_n=\partial\chi/dt=-v\,d\chi/d\xi=-(v/l)\partial\chi/dn$$
$$\approx-(v/l)(\chi_{n+1}-\chi_n),$$

$$\dot{\phi}_n\approx-(v/l)(\phi_{n+1}-\phi_n).$$

Here we neglected the higher-order finite increments; therefore, this approximation is restricted to the case of smooth enough solutions. The kinetic energy of the chain may now be expressed as

$$\mathcal{K}=\frac{1}{2}m\left\{\sum_{k=0}^{N}\dot{u}_{2k}^2+\sum_{n=0}^{N-1}\dot{u}_{2k+1}^2\right\}$$
$$=\frac{1}{2}m\left\{\sum_{k=0}^{N-1}[(\dot{\chi}_k-\dot{\phi}_k)^2+(\dot{\chi}_k+\dot{\phi}_k)^2]+\dot{u}_{2N}^2\right\}$$
$$=\frac{1}{2}m\left\{2\sum_{k=0}^{N-1}(\dot{\chi}_k^2+\dot{\phi}_k^2)+\dot{u}_{2N}^2\right\}$$
$$\approx\frac{mv^2}{l^2}\sum_{k=0}^{N-1}[(\chi_{k+1}-\chi_k)^2+(\phi_{k+1}-\phi_k)^2]+\frac{1}{2}m\dot{u}_{2N}^2.$$

Let us note that

$$\chi_{k+1}-\chi_k=\frac{1}{2}(u_{2k+3}+u_{2k+2}-u_{2k+1}-u_{2k})$$
$$=\frac{1}{2}(w_{2k+2}+2w_{2k+1}+w_{2k}),$$

$$\phi_{k+1}-\phi_k=\frac{1}{2}(u_{2k+3}-u_{2k+2}-u_{2k+1}+u_{2k})$$
$$=\frac{1}{2}(w_{2k+2}-w_{2k}),$$

then the chain Lagrangian can be written in the form

$$\mathcal{L}=-\mathcal{K}+\mathcal{P}$$
$$=-\frac{mv^2}{4l^2}\sum_{k=0}^{N-1}[(w_{2k+2}+2w_{2k+1}+w_{2k})^2+(w_{2k+2}-w_{2k})^2]-\frac{1}{2}m\dot{u}_{2N}^2+\sum_{k=1}^{N-2}[V_{1,\delta}(w_{2k})+V_{1,\delta}(w_{2k+1})+V_2(w_{2k}+w_{2k+1})]+\sum_{k=1}^{N-1}[V_2(w_{2k-1}+w_{2k})].$$

To find the dynamic state of a topological defect moving with given velocity, $s=v/v_0$, where $v_0=l\sqrt{C_2/m}$, a minimization problem is to be solved:

$$\mathcal{L}\rightarrow\min_{w_{2k},w_{2k+1}},\quad 1\leqslant k\leqslant N-2, \tag{67}$$

with boundary conditions (63) or (64).

The problems (63),(67), and (64),(67) have been solved numerically by conjugated gradient method. The dependence of the defect energy $E=E_{\pm}(s)-E_{\pm}(0)$ and its geometrical characteristics on dimensionless velocity s is illustrated by Fig. 7. The defect has a continuous subsonic velocity spectrum. The energy and the absolute value of amplitude monotonically increase, and the diameter monotonically decreases in line with the velocity increase.

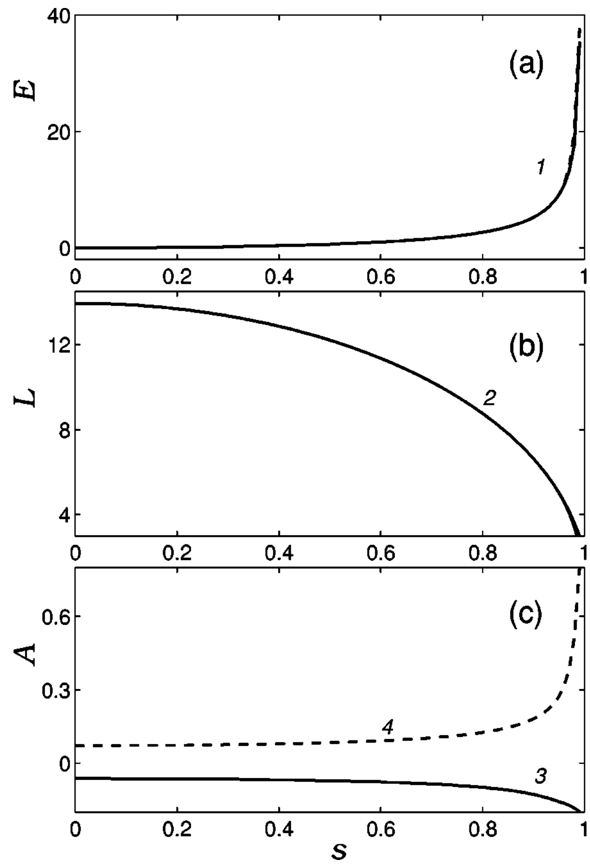

FIG. 7. The dependence of the defect energy relative to the energy of the stationary defect E (curve 1), diameter L, and amplitudes $A_{\pm}$ (curves 3, 4) on s for $a_1=1$, $a_2=3$, $b=6.5$, $c=3.5$, $\delta=0.4$, $\alpha=50$.

V. TRANSITION BETWEEN ALTERNATING AND INTERMEDIATE HOMOGENEOUS STATES

We have considered above the topological defects pertinent to the AUS. These defects are topological solitons that transfer the chain from one stationary state to another state with the same energy level. The existence of such solitons is the consequence of the symmetrical bistability of the chain, i.e., the availability of two equienergetic stationary states $\{+-\}$ and $\{-+\}$. The velocity spectrum of a defect is subsonic, and the defect's profile remains constant during motion.

In the system under consideration, in addition to stationary AUS's $\{+-\}$ and $\{-+\}$, stable stationary states energetically nonequivalent to them may be revealed. In this case, we are dealing with an asymmetric multistable system. It was shown in [6–8] that in asymmetric bistable *molecular* systems topological solitons may exist. Such solitons transfer the system from the ground uniform stationary state to a certain metastable dynamic state. A characteristic feature of such solitons is that they only can move with the unique velocity. Let us refer to such topological solitons as *metastable*, in contrast to those considered above. In this section we demonstrate that in the *atomic* system in question, in addition to conventional topological solitons (defects), metastable solitons may also exist.

A. Dynamic metastable stationary states

In the asymmetrical multistable chain under consideration, besides static stationary states, dynamic metastable stationary states may also exist. With the help of molecular variables introduced in Eq. (29) the system's Hamiltonian is expressed in the form

$$\mathcal{H}=\sum_n \{m(\dot{\chi}_n^2+\dot{\phi}_n^2)+V_{1,\delta}(2\phi_n)+V_{1,\delta}(\chi_{n+1}-\chi_n-\phi_{n+1}-\phi_n)+V_2(\chi_{n+1}-\chi_n-\phi_{n+1}+\phi_n)+V_2(\chi_{n+1}-\chi_n+\phi_{n+1}-\phi_n)\}. \tag{68}$$

In the AUS we have $\phi_n=r^-_{a,\delta}/2$, $\chi_n=nl+r^-_{a,\delta}/2$ (we could also shift the enumeration so that $r^+_{a,\delta}$ would stand instead of $r^-_{a,\delta}$, and vice versa). Therefore, for characterization of nonuniform (defective) alternating states it is convenient to introduce the relative displacement of the center of the nth molecule

$$r_n=\chi_n-(nl+r^-_{a,\delta}/2).$$

Then the Hamiltonian (68) may be rewritten in the form

$$\mathcal{H}=\sum_n \{m(\dot{r}_n^2+\dot{\phi}_n^2)+V_{1,\delta}(2\phi_n)+V_{1,\delta}(r_{n+1}-r_n+l-\phi_{n+1}-\phi_n)+V_2(r_{n+1}-r_n+l-\phi_{n+1}+\phi_n)+V_2(r_{n+1}-r_n+l+\phi_{n+1}-\phi_n)\}. \tag{69}$$

Let us find the metastable (intermediate) dynamic AUS of the chain. Suppose that a constant-profile wave is running with velocity v along the chain, then

$$r_n(t)=r(nl-vt), \quad \phi_n(t)=\phi(nl-vt),$$

$$\dot{r}_n(t)=-\frac{v}{l}(r_{n+1}-r_n), \quad \dot{\phi}_n(t)=-\frac{v}{l}(\phi_{n+1}-\phi_n).$$

Thus, the chain Lagrangian has the form

$$\mathcal{L}=\sum_n \left\{-m\frac{v^2}{l^2}[y_n^2+(\phi_{n+1}-\phi_n)^2]+V_{1,\delta}(2\phi_n)+V_{1,\delta}(y_n+l-\phi_{n+1}-\phi_n)+V_2(y_n+l-\phi_{n+1}+\phi_n)+V_2(y_n+l+\phi_{n+1}-\phi_n)\right\}, \tag{70}$$

where $y_n=r_{n+1}-r_n$.

Let $y_n\equiv y$, $\phi_n\equiv\phi$. Then the Lagrangian (70) is proportional to the following function:

$$\mathcal{F}(y,\phi,v)=-m\frac{v^2}{l^2}y^2+V_{1,\delta}(2\phi)+V_{1,\delta}(y+l-2\phi)+2V_2(y+l). \tag{71}$$

At any particular value of velocity v the metastable uniform state $\{y_v,\phi_v\}$ corresponds to the minimum of the function (71). This state and corresponding parameters may be found numerically by solving the minimization problem

$$\mathcal{F}_0(v)\equiv\mathcal{F}(y_v,\phi_v;v)=\min_{y,\phi}\mathcal{F}(y,\phi;v). \tag{72}$$

A metastable AUS coincides with the static AUS only for $v=0$, when $y=0$ and $\phi=r^-_{a,\delta}/2$.

B. Metastable topological soliton

Let us consider a topological soliton that describes the transition from the ground state to a metastable state. Such a transition can only occur if $\mathcal{F}_0$ for the metastable state equals the value of $\mathcal{F}$ for the ground state, i.e., if

$$\mathcal{F}_0(v)=\mathcal{F}_0(0). \tag{73}$$

Thus, the metastable topological soliton may only have a discrete spectrum of velocities. The velocity values may be found numerically as solutions of Eq. (73).

Suppose that Eq. (73) has a nontrivial solution $v=\overline{v}>0$. Then, to find the profile of the metastable soliton, it is sufficient to solve the minimization problem

$$\mathcal{L}=\sum_{n=1}^{N-1}\left\{-m\frac{\overline{v}^2}{l^2}[y_n^2+(\phi_{n+1}-\phi_n)^2]+V_{1,\delta}(2\phi_n)+V_{1,\delta}(y_n+l-\phi_{n+1}-\phi_n)+V_2(y_n+l-\phi_{n+1}+\phi_n)+V_2(y_n+l+\phi_{n+1}-\phi_n)\right\}\to\min_{y_2,\ldots,y_{N-1};\phi_2,\ldots,\phi_{N-1}} \tag{74}$$

with fixed boundary conditions

$$y_1=0, \quad \phi_1=r^-_{a,\delta}/2, \quad y_N=y_v, \quad \phi_N=\phi_N. \tag{75}$$

The boundary conditions on the left edge of the chain correspond to the ground uniform state $\{y_n\equiv0,\phi_n\equiv r^-_{a,\delta}/2,v=0\}$ and on the right edge to the metastable state $\{y_n\equiv y^-_{\overline{v}},\phi_n\equiv\phi^-_{\overline{v}},v=\overline{v}\}$.

The solution $\{y_n,\phi_n\}_{n=1}^N$ of the problem (74),(75) describes the soliton profile. The above numerical method of calculation of the soliton profile is an application of the principle of minimal action. It was used earlier in Refs. [18,19]. A necessary condition for this method is the smooth dependence of the soliton profile on the particle number n. Formal solutions to the problem (74),(75) that do not depend smoothly on n do not make physical sense.

The problem (74),(75) was solved by a conventional method of conjugated gradients. The initial approximation profile was chosen in the form

$$\phi_n=A_1+B_1\tanh[(n-N/2)\mu],$$

$$y_n=A_2+B_2\tanh[(n-N/2)\mu],$$

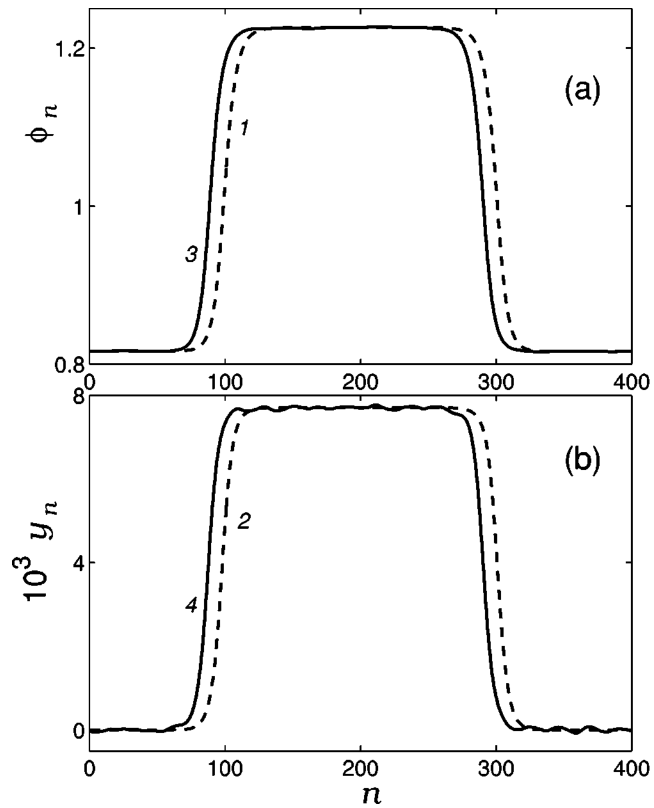

FIG. 8. Profiles of two metastable topological solitons of different signs for $\tau=0$ (curves 1, 2) and $\tau=21\,698$ (curves 3, 4). The velocity of solitons $s=0.4609$; chain parameters are $a_1=1$, $a_2=3$, $b=4.899$, $c=2$, $\alpha=1$, $\delta=$ 0.4, and $\alpha=50$.

where $A_1=(\phi_1+\phi_N)/2$, $A_2=(y_1+y_N)/2$, $B_1=\phi_N-A_1$, $B_2=y_N-A_2$. The soliton center's position and radius are defined by analogy with Eqs. (65) and (66) as

$$P=\sum_{n=1}^{N-1} n(\phi_{n+1}-\phi_n)/(\phi_N-\phi_1),$$

$$R=\left\{\sum_{n=1}^{N-1}(p-n)^2(\phi_{n+1}-\phi_n)/(\phi_N-\phi_1)\right\}^{1/2}.$$

The number of nodes N for the solution of the problem (74) must be taken approximately ten times larger than the soliton diameter $L=2R+1$. Then it is guaranteed that the boundary conditions will not influence the soliton shape.

Let us consider an example. In the chain with parameters $a_1=1$, $a_2=3$, $c=2$, $\delta=0.4$, $C_1=1$, $\alpha=50$, $b=4.899$ the metastable topological soliton has dimensionless velocity $s=\overline{v}/v_0=0.4609$ and diameter $L=18.06$. A plot for a pair of solitons of different signs is shown in Fig. 8. The first and last quarters of the chain are in the ground uniform state $\{y_n\equiv 0,\phi_n\equiv r^-_{a,\delta}/2\}$ ($r^-_{a,\delta}=1.633$, $r^+_{a,\delta}=3.262$, $l=r^-_{a,\delta}+r^+_{a,\delta}=4.896$), and the rest of the chain is in the metastable state $\{y_n\equiv y_v=7.703\times 10^{-3},\ \phi_n\equiv\phi_v=1.226,\ s=0.4609\}$.

Let us remember that the variable $y_n=(x_{2n+3}+x_{2n+2}-x_{2n+1}-x_{2n})/2-l$ characterizes the variation of the molecular chain period, and the variable $\phi_n=(x_{2n+1}-x_{2n})/2$ is the half-length of odd bonds. Note that in the metastable state the lengths of odd and even bonds coincide: $x_{2n+1}-x_{2n}=2\phi_v=l+y_v-2\phi_v=x_{2n+2}-x_{2n+1}$. Thus, the metastable state is topologically equivalent to the uniform state $\{--\}$.

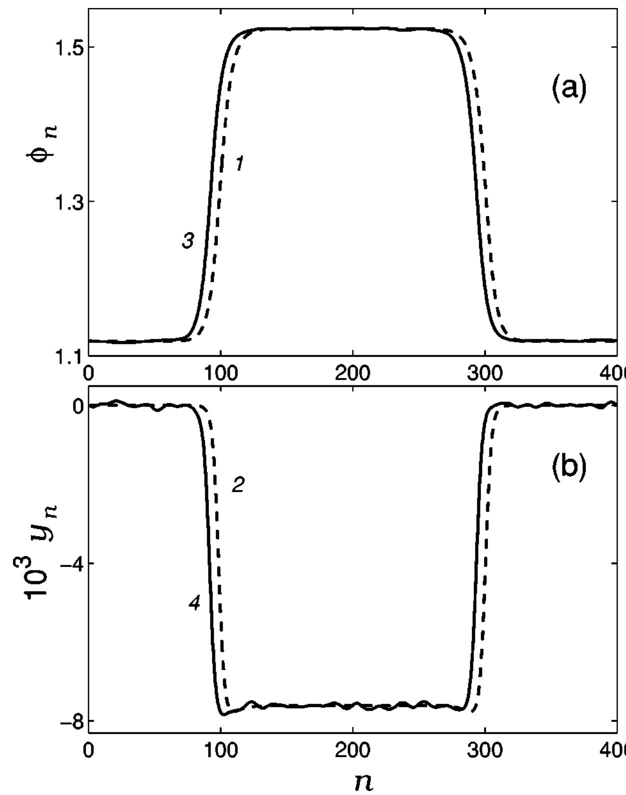

FIG. 9. Profiles of two metastable topological solitons of different signs for $\tau=0$ (curves 1, 2) and $\tau=12\,906$ (curves 3, 4).The velocity of solitons $s=0.7748$; chain parameters are $a_1=1$, $a_2=3$, $b=6.11$, $c=3.5$, $\alpha=1$, $\delta=$ 0.4, and $\alpha=100$.

By analogy, in the chain with parameters $a_1=1$, $a_2=3$, $c=3.5$, $\delta=0.4$, $C_1=1$, $\alpha=100$, $b=6.11$ the metastable topological soliton has the velocity $s=0.7748$ and diameter $L=18.21$. A graph for a pair of different sign solitons is shown in Fig. 9. The first and last quarters of the chain are in the ground uniform state $\{y_n\equiv 0,\phi_n\equiv r^-_{a,\delta}/2\}$ ($r^-_{a,\delta}=2.238, r^+_{a,\delta}=3.866, l=r^-_{a,\delta}+r^+_{a,\delta}=6.104$), and the rest of the chain is in the metastable state $\{y_n\equiv y_v=-7.613\times 10^{-3},\phi_n\equiv\phi_v=1.524, v=\overline{v}=0.7748\}$. Here again in the metastable state the lengths of odd and even bonds coincide: $2\phi_v=l+y_v-2\phi_v$.

It can be concluded that the metastable topological soliton, the existence of which is connected with asymmetrical bistability of the molecular system, i.e., the existence of two stable uniform states $\{-+\}$ and $\{--\}$ with different energies, describes the system's transformation from the ground uniform state $\{-+\}$ to the dynamic metastable uniform state, which is topologically equivalent to the uniform state $\{--\}$.

VI. NUMERICAL MODELING OF SOLITON DYNAMICS

To examine the stability of the solitons revealed in Sec. IV, we have studied their motion by molecular dynamics.

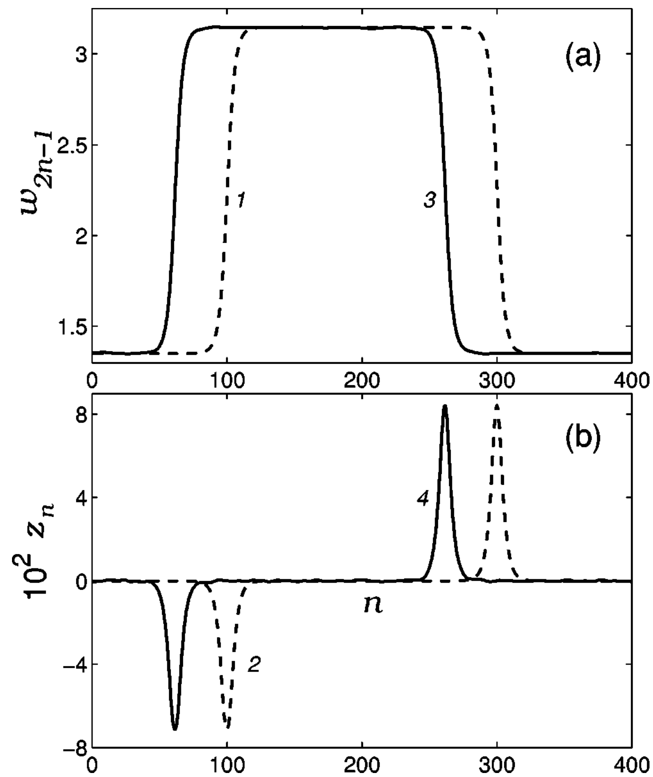

FIG. 10. Profiles of two topological defects of different signs in a cyclic chain for $\tau=0$ (curves 1, 2) and $\tau=20\,000$ upon passing 9963 chain units (curves 3, 4). The initial velocity of defects $s=0.5$; chain parameters are $a_1=1$, $a_2=3$, $b=4.5$, $c=2$, $\delta=0.4$, and $\alpha=50$.

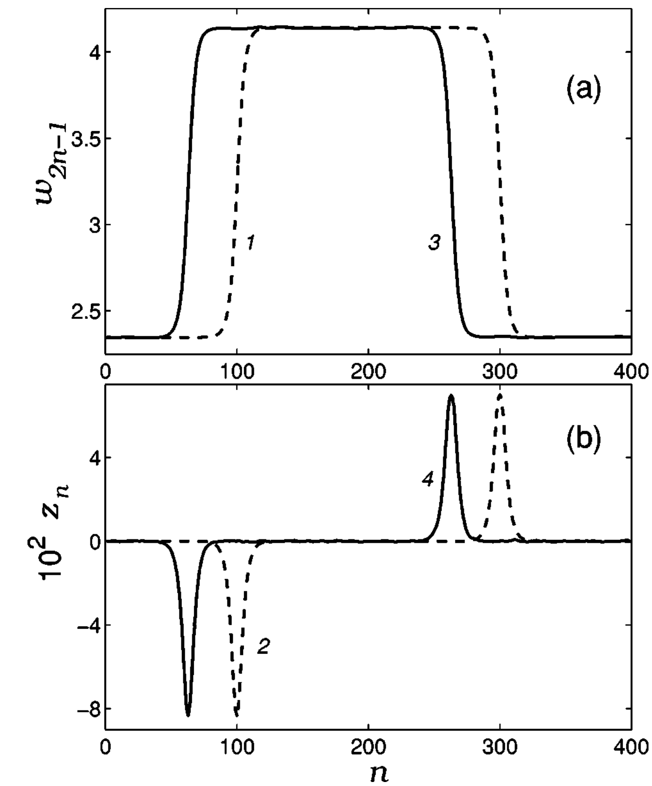

FIG. 11. Profiles of two topological defects of different signs in a cyclic chain for $\tau=0$ (curves 1, 2) and $\tau=20\,000$ upon passing 9937 chain units (curves 3, 4).The initial velocity of defects $s=0.5$; chain parameters are $a_1=1$, $a_2=3$, $b=6.5$, $c=3.5$, $\delta=$ 0.4, and $\alpha=50$.

A. Numerical modeling of the dynamics of topological defects

Let us consider first of all the dynamics of topological solitons describing the transition between alternating states $\{+-\}$ and $\{-+\}$. Using the system's Hamiltonian

$$\mathcal{H}=\sum_n \left\{\frac{1}{2}m(\dot{u}_{2n}^2+\dot{u}_{2n-1}^2)+V_1(w_{2n})+V_1(w_{2n+1}) + V_2(w_{2n}+w_{2n+1})+V_2(w_{2n+1}+w_{2n})\right\},$$

it is easy to derive the equations of motion,

$$m\ddot{u}_{2n}=V_1'(w_{2n})-V_1'(w_{2n-1})+V_2'(w_{2n}+w_{2n+1}) -V_2'(w_{2n-2}+w_{2n-1}),$$

$$m\ddot{u}_{2n+1}=-V_1'(w_{2n})+V_1'(w_{2n+1})+V_2'(w_{2n+1}+w_{2n+2}) -V_2'(w_{2n-1}+w_{2n}).$$

Then

$$m\ddot{w}_{2n}=m(\ddot{u}_{2n+1}-\ddot{u}_{2n}) =-2S_{n,1}+S_{n,2}+S_{n-1,2}+S_{n-1,3}-S_{n,3}+S_{n,4}-S_{n-1,4}, \tag{76}$$

$$m\ddot{\omega}_n=m(\ddot{u}_{2n+2}-\ddot{u}_{2n}) =S_{n+1,1}-S_{n,1}+S_{n-1,2}-S_{n,2}+S_{n+1,3}-2S_{n,3}+S_{n-1,3}, \tag{77}$$

where

$$\omega_n=w_{2n}+w_{2n+1},\quad S_{n,1}=V_1'(w_{2n}),\quad S_{n,2}=V_1'(w_{2n+1}),$$

$$S_{n,3}=V_2'(w_{2n}+w_{2n+1}),\quad S_{n,4}=V_2'(w_{2n+1}+w_{2n+2}).$$

In order to simulate the dynamics of topological defects in an infinite chain, consider the movement of a pair of defects of different signs in a cyclic chain of $N=400$ particles. Impose periodical conditions $u_1\equiv u_{N+1}$ on Eqs. (76) and (77) and take the initial conditions that correspond to the distance $N/2$ between the defects (see Figs. 10 and 11)

$$w_{2n}(0)=w_{2n}^0,\quad \omega_n(0)=\omega_n^0,\quad n=1,\dots,N,$$

$$w_{2n}'(0)=-s_1(w_{2(n+1)}^0-w_{2n}^0),\quad \omega_n'(0)=-s_1(\omega_{n+1}^0-\omega_n^0),$$

$$n=1,\dots,N/2, \tag{78}$$

$$w_{2n}'(0)=-s_2(w_{2(n+1)}^0-w_{2n}^0),\quad \omega_n'(0)=-s_2(\omega_{n+1}^0-\omega_n^0),$$

$$n=N/2+1,\dots,N.$$

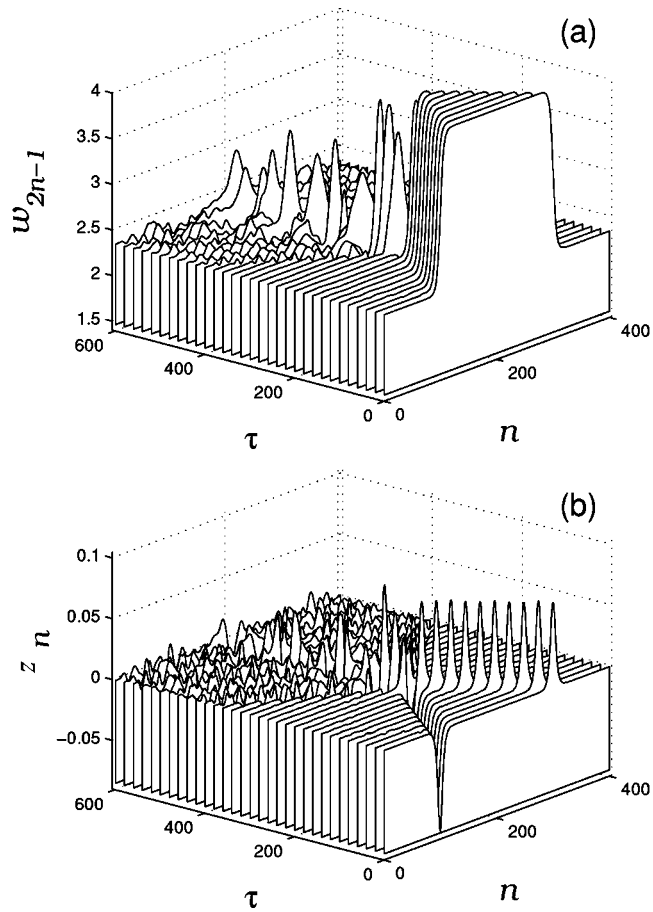

FIG. 12. Appearance of a breatherlike nonlinear vibration at the impact of two topological defects of different signs. The boundary condition corresponds to phonon absorption at the chain edges. The initial velocity of defects $s_1=-s_2=0.5$; chain parameters are $a_1=1$, $a_2=3$, $b=6.5$, $c=3.5$, $\delta=0.4$, and $\alpha=50$.

Here $\{w^0_{2n},\omega^0_n\}$ is the defect profile calculated by solving problem (67); s_1 and s_2 are dimensionless velocities of the first and second defects. To simplify the derivations, dimensionless time $\tau=tv_0/l$ is introduced; the prime denotes the derivative $d/d\tau$.

Thus, one should solve a system of equations

$$c_3w''_{2n}=-2S_{n,1}+S_{n,2}+S_{n-1,2}+S_{n-1,3}-S_{n,3}+S_{n,4}-S_{n-1,4},$$
$$c_3\omega''_n=S_{n+1,1}-S_{n,1}+S_{n-1,2}-S_{n,2}+S_{n+1,3}-2S_{n,3}+S_{n-1,3},\quad n=1,2,\ldots,N \tag{79}$$

with initial conditions (78), where $c_3=mv_0^2/l^2$.

The system (79) was solved by the conventional Runge-Kutta method of fourth order accuracy. It was found that the topological defects exhibit solitonic dynamics, i.e., they move with constant velocity and profile. For example, for $\alpha=50$, $s_1=s_2=0.5$, $\tau=20\,000$ the defects passed 9963 chain units (computed $s=0.498$; see Fig. 10) for the set (60) of chain parameters, and 9937 chain units (computed $s=0.497$; see Fig. 11) for the set (61). The profiles of the defects in the initial and final moments perfectly coincide.

Figure 12 demonstrates the effect of the impact of two different-sign defects running in opposite directions ($s_1=0.5$, $s_2=-0.5$). The impact leads to recombination of the defects. As a result, fast relaxing nonlinear oscillations of the breather type occur. The oscillations are accompanied by phonon radiation.

B. Numerical modeling of the dynamics of metastable topological solitons

Consider now the dynamics of metastable topological solitons. The Hamiltonian (69) yields the system of equations of motion

$$2m\ddot{\phi}_n=-2S_{1,n}+S_{2,n}+S_{2,n-1}-S_{3,n}+S_{3,n-1}+S_{4,n}-S_{4,n-1},$$
$$2m\ddot{r}_n=S_{2,n}-S_{2,n-1}+S_{3,n}-S_{3,n-1}+S_{4,n}-S_{4,n-1},$$
$$n=0,\pm1,\pm2,\ldots, \tag{80}$$

where

$$S_{1,n}=V'_1(2\phi_n),\quad S_{2,n}=V'_1(y_n+l-\phi_{n+1}-\phi_n),$$
$$S_{3,n}=V'_2(y_n+l-\phi_{n+1}-\phi_n),$$
$$S_{4,n}=V'_2(y_n+l+\phi_{n+1}-\phi_n).$$

Using relative displacements $y_n=r_{n+1}-r_n$, Eq. (80) may be rewritten as

$$2m\ddot{\phi}_n=-2S_{1,n}+S_{2,n}+S_{2,n-1}-S_{3,n}+S_{3,n-1}+S_{4,n}-S_{4,n-1},$$
$$2m\ddot{y}_n=S_{2,n+1}-2S_{2,n}+S_{2,n-1}+S_{3,n+1}-2S_{3,n}+S_{3,n-1}+S_{4,n+1}-2S_{4,n}+S_{4,n-1},$$
$$n=0,\pm1,\pm2,\ldots.$$

Introduce again the dimensionless time τ and consider the dynamics of a kink-antikink pair in a finite chain with periodic boundary conditions. Then the following system of equations must be integrated numerically:

$$c_4\phi''_n=-2S_{1,n}+S_{2,n}+S_{2,n-1}-S_{3,n}+S_{3,n-1}+S_{4,n}-S_{4,n-1},$$
$$c_4y''_n=S_{2,n+1}-2S_{2,n}+S_{2,n-1}+S_{3,n+1}-2S_{3,n}+S_{3,n-1}+S_{4,n+1}-2S_{4,n}+S_{4,n-1}, \tag{81}$$
$$n=1,2,\ldots,N,$$

where $c_4=2mv_0^2/l^2$.

Equation (81) was integrated by the conventional Runge-Kutta method of fourth order accuracy. In the chain with parameters $a_1=1$, $a_2=3$, $c=2$, $\delta=0.4$, $\alpha=50$, $b=4.899$ the soliton had the dimensionless velocity $s=0.4609$. At this velocity the kink-antikink pair must pass $N_p=10\,000$ chain units for $\tau=N_p/s=21698$. Figure 8 presents the soliton profiles at $\tau=0$ and $\tau=21\,698$. In the numerical experiment the

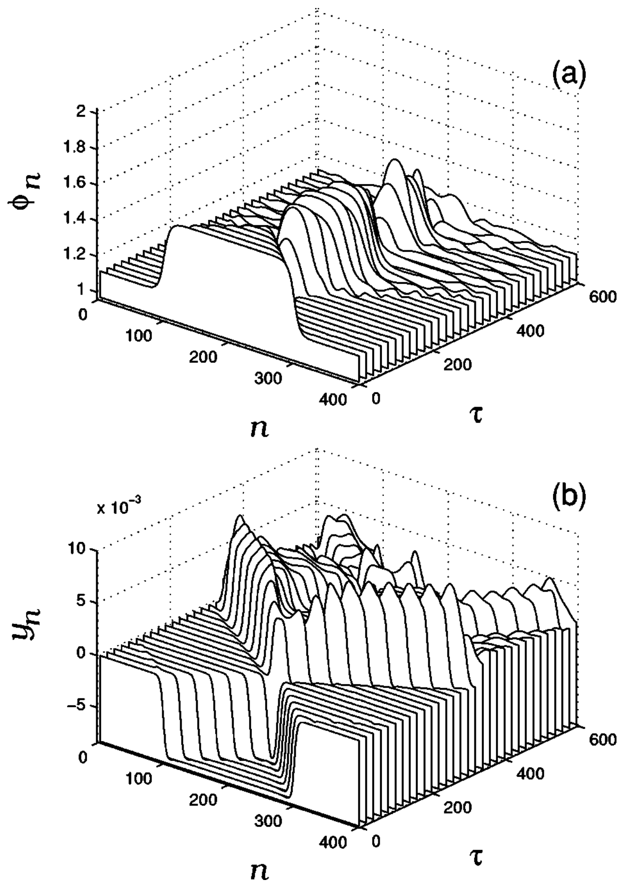

FIG. 13. Impact of two metastable topological solitons of different signs in a chain with parameters $a_1=1$, $a_2=3$, $b=6.11$, $c=3.5$, $\delta=0.4$, and $\alpha=100$. The boundary condition corresponds to phonon absorption on the chain edges.

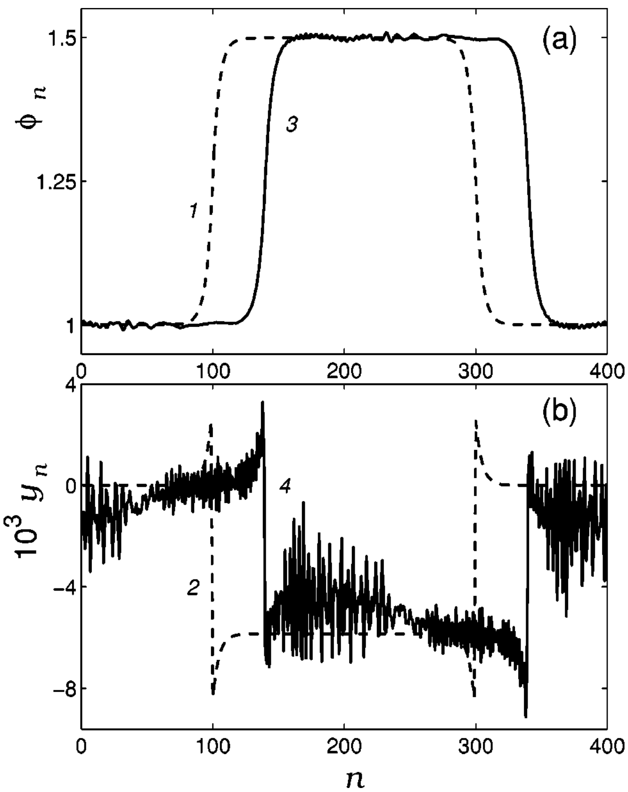

FIG. 14. Dynamics of two metastable topological solitons of different signs in a chain with parameters $a_1=1$, $a_2=3$, $b=6.008$, $c=3.5$, $\delta=0.01$, and $\alpha=100$. Curves 1, 2 give the soliton profiles for $\tau=0$; curves 3, 4 correspond to $\tau=250$.

solitons have passed $\overline{N_p}=9990$ chain units, which corresponds to $\overline{s}=0.4604$. As is seen, the final profiles perfectly coincide with the initial ones.

Now take the parameters $a_1=1$, $a_2=3$, $c=3.5$, $\delta=0.4$, $\alpha=100$, $b=6.11$, then $s=0.7749$, $\tau=10\,000/s=12\,906$. The soliton profiles are plotted for $\tau=0$ and $\tau=12\,906$ in Fig. 9. In reality, the solitons passed $\overline{N_p}=9993$ chain units during this time, moving with constant velocity $\overline{s}=0.7743$.

The picture of impact of two different-sign solitons in a chain with phonon absorption on its edges is presented in Fig. 13. The impact is inelastic and leads to phonon irradiation. Recombination of topological solitons takes place, and then the entire chain transfers to the ground uniform state.

At weak enough smoothening of the piecewise-parabolic NN potential (small δ) the topological solitons are no longer dynamically stable. Thus, at $a_1=1$, $a_2=3$, $c=3.5$, $\delta=0.01$, $\alpha=100$, $b=6.008$ we obtain $s=0.3844$, $L=14.08$. Figure 14 shows the kink-antikink pair profiles for $\tau=0$ (dashed line) and $\tau=251$ (solid line). The solitons have passed 40 chain units and stopped. Their movement was accompanied by intense phonon irradiation. Therefore, the smoothness of the particle interaction potential is a necessary condition for the dynamic stability of topological solitons.

VII. CONCLUSIONS

It was shown that stable topological solitons may exist in a wide class of *one-component* (atomic) chains with both degenerate and even *nondegenerate* gradient-type potentials. Such solitons may correspond to movement of localized structural defects in the chain or to transition of the entire chain to a metastable dynamic state. The motion of a defect may be considered as an elementary event of structural transitions or chemical reactions in one-dimensional atomic crystals or conformational transitions in linear macromolecules. In systems with nondegenerate potential, the solitons that transfer the system to a metastable dynamic state can move with the only possible value of velocity, which is found to be subsonic. For both types of solitons, their profile remains constant during motion and phonon radiation is absent as long as the nearest-neighbor interaction potential is smooth enough. The interaction between solitons turns out to be inelastic, and the collision of two solitons of different signs leads to their recombination.

ACKNOWLEDGMENTS

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APPENDIX

(1) Consider an algebraic equation with constant real coefficients,

$$B_4\lambda^4+B_2\lambda^2+B_0=0. \tag{A1}$$

Provided that $B_2\neq 0$ and $B_4\neq 0$, its roots are given by

$$\lambda_{1,2}=\sqrt{-\frac{1}{2}q_1(1\pm\sqrt{1-4q_2})},\quad \lambda_3=-\lambda_1,\quad \lambda_4=-\lambda_2, \tag{A2}$$

where

$$q_1=B_2/B_4,\quad q_2=B_0B_4/B_2^2. \tag{A3}$$

If $|q_2|\ll 1$, then the following asymptotic estimate is valid:

$$\lambda^2=-\frac{1}{2}q_1\{1\pm[1-2q_2-2q_2^2+o(q_2^2)]\},$$

$$\lambda_1\approx\sqrt{-q_1q_2(1+q_2)},\quad \lambda_2\approx\sqrt{-q_1(1-q_2)}. \tag{A4}$$

If $|B_4|\to 0$ with B_2 and B_0 fixed, then $|\lambda_{2,4}|\to\infty$ and $|\lambda_{1,3}|\to\sqrt{-q_1q_2}=\sqrt{-B_0/B_2}$.

(2) Consider an ordinary fourth-order differential equation with constant real coefficients and a nonlinear term,

$$B_4y^{(IV)}+B_2y''+B_0y+A_1\mathrm{sgn}(y)+A_2=0, \tag{A5}$$

with boundary conditions

$$\lim_{x\to+\infty}y(x)=y_0,\quad |y_0|<\infty;\quad |y(x)|<\infty,\quad x\to-\infty. \tag{A6}$$

The coefficients B_i are assumed to be such that $B_2\neq 0$, $B_4\neq 0$, $q_1<0$, and $0<q_2<1/4$, where $q_{1,2}$ are defined by Eq. (A3). The characteristic equation for the linear part of Eq. (A5) is Eq. (A1), its roots being given by Eq. (A2). It is easy to see that all the roots of Eq. (A1) are real, and the positive roots $\lambda_{1,2}$ may be chosen so that

$$0<\lambda_1<\lambda_2. \tag{A7}$$

The problem is to find such functions $y(x)$ satisfying Eqs. (A5) and (A6) that $y(x)$ is at least three times continuously differentiable and $y^{(IV)}(x)$ is bounded for any $x\in(-\infty,+\infty)$.

The problem (A5),(A6) is overdefined, and a necessary condition for a solution to exist is

$$y_0=-[\mathrm{sgn}(y_0)A_1+A_2]/B_0. \tag{A8}$$

It is noteworthy that it is sufficient to solve the problem for $y_0>0$. Indeed, let us find the solution Y for $Y_0=-a<0$, provided that the solution y for $y_0=a>0$ is known as a function of argument x and parameters A_i, B_i, y_0. We introduce an auxiliary function, $\tilde{y}=-y$. This function satisfies Eq. (A5) with the only change, $A_2\to -A_2$. The boundary conditions for $\tilde{y}(x)$ coincide with Eq. (A6), and $\tilde{y}_0=-y_0=Y_0$. Therefore, Y may be expressed as a function of argument x, the limit value y_0, and coefficient A_2:

$$Y(x;Y_0,-A_2)=-y(x;y_0,A_2).$$

In general, for arbitrary y_0, A_2,

$$y(x;y_0,A_2)=\mathrm{sgn}(y_0)y(x;|y_0|,\mathrm{sgn}(y_0)A_2). \tag{A9}$$

(3) Suppose that $y_{1,0}(x)$ is a solution to Eq. (A5) such that $y_{1,0}(x)=0$ for $x=-d_1$ and $y_{1,0}(x)>0$ for $-d_1<x<\infty$, d_1 being a constant. The general form of $y_{1,0}(x)$ is as follows:

$$y_{1,0}(x)=c_{0,0}^{(1)}+c_{1,0}^{(1)}e^{-\lambda_1x}+c_{2,0}^{(1)}e^{-\lambda_2x}+c_{3,0}^{(1)}e^{\lambda_1x}+c_{4,0}^{(1)}e^{\lambda_2x},$$

where $c_{i,0}^{(1)}$ are some constants. Make a shift of the variable x: $x_1=x+d_1$, then the function $y_{1,0}(x)$ is transformed into $y_{1,1}(x_1)$ that may be written down as

$$y_{1,1}(x_1)=c_{0,1}^{(1)}+c_{1,1}^{(1)}e^{-\lambda_1x_1}+c_{2,1}^{(1)}e^{-\lambda_2x_1}+c_{3,1}^{(1)}e^{\lambda_1x_1}+c_{4,1}^{(1)}e^{\lambda_2x_1}, \tag{A10}$$

according to the following rules:

$$c_{0,1}^{(1)}=c_{0,0}^{(1)},\quad c_{1,1}^{(1)}=c_{1,0}^{(1)}e^{\lambda_1d_1},\quad c_{2,1}^{(1)}=c_{2,0}^{(1)}e^{\lambda_2d_1},$$

$$c_{3,1}^{(1)}=c_{3,0}^{(1)}e^{-\lambda_1d_1},\quad c_{4,1}^{(1)}=c_{4,0}^{(1)}e^{-\lambda_2d_1}.$$

Now $y_{1,1}(0)=0$.

Let us find such function $y_{2,1}(x_1)$ satisfying Eq. (A5),

$$y_{2,1}(x_1)=c_{0,1}^{(2)}+c_{1,1}^{(2)}e^{-\lambda_1x_1}+c_{2,1}^{(2)}e^{-\lambda_2x_1}+c_{3,1}^{(2)}e^{\lambda_1x_1}+c_{4,1}^{(2)}e^{\lambda_2x_1}$$

that it is defined within a certain region $-d_2\leqslant x_1\leqslant 0$, $d_2>0$; $y_{2,1}(-d_2)=y_{2,1}(0)=0$, $y_{2,1}(x_1)<0$ for $-d_2<x_1<0$, and the first three derivatives of $y_{2,1}$ for $x_1\to -0$ are equal to corresponding derivatives of $y_{1,1}$ for $x_1\to +0$. The latter conditions may be expressed in the following form:

$$\lambda_1(-c_{1,1}^{(2)}+c_{3,1}^{(2)}+c_{1,1}^{(1)}-c_{3,1}^{(1)})+\lambda_2(-c_{2,1}^{(2)}+c_{4,1}^{(2)}+c_{2,1}^{(1)}-c_{4,1}^{(1)})=0, \tag{A11}$$

$$\lambda_1^2(c_{1,1}^{(2)}+c_{3,1}^{(2)}-c_{1,1}^{(1)}-c_{3,1}^{(1)})+\lambda_2^2(c_{2,1}^{(2)}+c_{4,1}^{(2)}-c_{2,1}^{(1)}-c_{4,1}^{(1)})=0, \tag{A12}$$

$$\lambda_1^3(-c_{1,1}^{(2)}+c_{3,1}^{(2)}+c_{1,1}^{(1)}-c_{3,1}^{(1)})+\lambda_2^3(-c_{2,1}^{(2)}+c_{4,1}^{(2)}+c_{2,1}^{(1)}-c_{4,1}^{(1)})=0. \tag{A13}$$

Equations (A11) and (A13) may be considered as a linear system of equations respective to the sums in parentheses. For $\lambda_1\neq\lambda_2$ the only solution is

$$c_{1,1}^{(2)}-c_{3,1}^{(2)}=c_{1,1}^{(1)}-c_{3,1}^{(1)}, \tag{A14}$$

$$c_{2,1}^{(2)}-c_{4,1}^{(2)}=c_{2,1}^{(1)}-c_{4,1}^{(1)}. \tag{A15}$$

Now we can substitute Eqs. (A14) and (A15) into Eq. (A12) to obtain

$$c_{2,1}^{(2)}-c_{2,1}^{(1)}=-\frac{\lambda_1^2}{\lambda_2^2}(c_{1,1}^{(2)}-c_{1,1}^{(1)}). \tag{A16}$$

Since $y_{1,1}(x_1)\geqslant 0$ and $y_{2,1}(x_1)\leqslant 0$ within their range of definition, it is easy to see from Eq. (A5) that

$$c_{0,1}^{(1)}=-(A_1+A_2)/B_0,\quad c_{0,1}^{(2)}=(A_1-A_2)/B_0. \tag{A17}$$

Moreover, $y_{1,1}(0)=y_{2,1}(0)=0$, therefore,

$$\sum_{i=0}^{4} c_{i,1}^{(1)}=\sum_{i=0}^{4} c_{i,1}^{(2)}=0. \tag{A18}$$

With the help of Eqs. (A14)–(A18) we perform the following transformations:

$$\sum_{i=0}^{4} c_{i,1}^{(2)}=c_{0,1}^{(2)}+c_{1,1}^{(2)}+\left[c_{2,1}^{(2)}-\frac{\lambda_1^2}{\lambda_2^2}(c_{1,1}^{(2)}-c_{1,1}^{(1)})\right]+[c_{1,1}^{(2)}-c_{1,1}^{(1)}$$
$$+c_{3,1}^{(1)}]+\left[c_{4,1}^{(2)}-\frac{\lambda_1^2}{\lambda_2^2}(c_{1,1}^{(2)}-c_{1,1}^{(1)})\right]$$
$$=c_{0,1}^{(2)}+2(c_{1,1}^{(2)}-c_{1,1}^{(1)})\left(1-\frac{\lambda_1^2}{\lambda_2^2}\right)+\sum_{i=1}^{4} c_{i,1}^{(1)}$$
$$=2(c_{1,1}^{(2)}-c_{1,1}^{(1)})\left(1-\frac{\lambda_1^2}{\lambda_2^2}\right)+(c_{0,1}^{(2)}-c_{0,1}^{(1)})=0.$$

This leads to

$$c_{1,1}^{(2)}-c_{1,1}^{(1)}=-\Lambda_1 A_1/B_0,\quad \Lambda_1=(1-\lambda_1^2/\lambda_2^2)^{-1}. \tag{A19}$$

Substitution of Eq. (A16) into Eq. (A19) yields

$$c_{2,1}^{(2)}-c_{2,1}^{(1)}=-\Lambda_2 A_1/B_0,\quad \Lambda_2=(1-\lambda_2^2/\lambda_1^2)^{-1}. \tag{A20}$$

Now we shift the x variable once again according to $x_2=x_1+d_2$, thus we transform $y_{2,1}(x_1)$ into $y_{2,2}(x_2)$, and then repeat the steps starting with Eq. (A10). It is easy to define the functions $y_{3,2}(x_2)$, $y_{4,3}(x_3)$, $\ldots,y_{n+1,n}(x_n)$ and $y_{3,3}(x_2)$, $y_{4,4}(x_3)$, $\ldots,y_{n,n}(x_n)$ such that every such function satisfies Eq. (A5) and

$$y_{k+1,k}(-d_{k+1})=y_{k+1,k}(0)=0,$$
$$\mathrm{sgn}(y_{k+1,k}(x_k))=(-1)^k\quad\text{for}\quad -d_{k+1}<x_k<0,$$
$$y_{k+1,k+1}(x_{k+1})\equiv y_{k+1,k}(x_k),$$
$$x_k=d_k+x_{k-1}=\cdots=\sum_{j=1}^{k} d_j+x,$$

where $k>0$ and $d_j>0$ for $j>1$. Let us introduce new variables

$$\omega_1=-\Lambda_1 A_1/B_0,\quad \omega_2=-\Lambda_2 A_1/B_0, \tag{A21}$$

then the relationships for the coefficients $c_{i,j}^{(k)}$, $k>0$, may be obtained by analogy with Eqs. (A19) and (A20) and with the aid of Eqs. (A14) and (A15) in the following form:

$$c_{0,j}^{(k)}=[(-1)^k A_1-A_2]/B_0\quad\text{for any}\quad j, \tag{A22}$$

$$c_{1,k}^{(k+1)}-c_{1,k}^{(k)}=c_{3,k}^{(k+1)}-c_{3,k}^{(k)}=(-1)^{k+1}\omega_1, \tag{A23}$$

$$c_{2,k}^{(k+1)}-c_{2,k}^{(k)}=c_{4,k}^{(k+1)}-c_{4,k}^{(k)}=(-1)^{k+1}\omega_2, \tag{A24}$$

$$c_{1,k}^{(k)}=c_{1,k-1}^{(k)}e^{\lambda_1 d_k}=c_{1,k-2}^{(k)}e^{\lambda_1(d_k+d_{k-1})}=\cdots$$
$$=c_{1,0}^{(k)}\exp\left(\lambda_1\sum_{j=1}^{k} d_j\right), \tag{A25}$$

$$c_{2,k}^{(k)}=c_{2,k-1}^{(k)}e^{\lambda_2 d_k}=\cdots=c_{2,0}^{(k)}\exp\left(\lambda_2\sum_{j=1}^{k} d_j\right), \tag{A26}$$

$$c_{3,k}^{(k)}=c_{3,k-1}^{(k)}e^{-\lambda_1 d_k}=\cdots=c_{3,0}^{(k)}\exp\left(-\lambda_1\sum_{j=1}^{k} d_j\right), \tag{A27}$$

$$c_{4,k}^{(k)}=c_{4,k-1}^{(k)}e^{-\lambda_2 d_k}=\cdots=c_{4,0}^{(k)}\exp\left(-\lambda_2\sum_{j=1}^{k} d_j\right). \tag{A28}$$

Note that $k>0$ throughout Eqs. (A22)–(A28).

Let us express $c_{1,k}^{(k+1)}$ through $c_{1,0}^{(1)}$ with the help of Eqs. (A23) and (A25). We subsequently obtain

$$c_{1,k}^{(k+1)}=(-1)^{k+1}\omega_1+c_{1,k}^{(k)}=(-1)^{k+1}\omega_1+e^{\lambda_1 d_k}c_{1,k-1}^{(k)}=\cdots$$
$$=\omega_1\{(-1)^{k+1}+e^{\lambda_1 d_k}[(-1)^k+\cdots+e^{\lambda_1 d_2}(1$$
$$+e^{\lambda_1 d_1}\omega_1^{-1}c_{1,0}^{(1)})\cdots]\}. \tag{A29}$$

An analogous relationship for $c_{2,k}^{(k+1)}$ is obtained from Eq. (A29) by replacements $(\omega_1\to\omega_2,\lambda_1\to\lambda_2)$; for $c_{3,k}^{(k+1)}$ by replacement $(\lambda_1\to-\lambda_1)$, and for $c_{4,k}^{(k+1)}$ by replacements $(\omega_1\to\omega_2,\lambda_1\to-\lambda_2)$.

Suppose now that the solution $y_{n+1,n}(x_n)$ is valid up to $x_n\to-\infty$ (this corresponds to $d_{n+1}\to\infty$). According to boundary conditions (A6), $y_{n+1,n}(x_n)$ must be limited, therefore, the coefficients $c_{1,n}^{(n+1)}=c_{2,n}^{(n+1)}=0$. Using this consideration and Eq. (A29), we are able to express $c_{1,0}^{(1)}$ as follows:

$$c_{1,0}^{(1)}=\omega_1 e^{-\lambda_1 d_1}(-1+e^{-\lambda_1 d_2}\{1+\cdots+e^{-\lambda_1 d_{n-1}}[(-1)^{n-1}$$
$$+e^{-\lambda_1 d_n}(-1)^n]\cdots\}). \tag{A30}$$

The equation for $c_{2,0}^{(1)}$ is obtained by the aforementioned replacements. In particular, for $n=1$

$$c_{1,0}^{(1)}=-\omega_1 e^{-\lambda_1 d_1},\quad c_{1,0}^{(1)}=-\omega_2 e^{-\lambda_2 d_1}. \tag{A31}$$

Substitution of Eq. (A30) into (A29) and use of Eq. (A25) yield

$$c_{1,k}^{(k)}=\omega_1((-1)^k+e^{-\lambda_1 d_{k+1}}\{(-1)^{k+1}+\cdots+e^{-\lambda_1 d_{n-1}}\times[(-1)^{n-1}+e^{-\lambda_1 d_n}(-1)^n]\cdots\}). \quad (A32)$$

By analogy,

$$c_{2,k}^{(k)}=\omega_2((-1)^k+e^{-\lambda_2 d_{k+1}}\{(-1)^{k+1}+\cdots+e^{-\lambda_1 d_{n-1}}\times[(-1)^{n-1}+e^{-\lambda_2 d_n}(-1)^n]\cdots\}). \quad (A33)$$

Boundary conditions (A6) with account of Eq. (A7) require that $c_{3,0}^{(1)}=c_{4,0}^{(1)}=0$; therefore, we can obtain similar expressions for $c_{3,k}^{(k)}$, $c_{4,k}^{(k)}$ by analogy with Eq. (A29):

$$c_{3,k}^{(k)}=\omega_1 e^{-\lambda_1 d_k}\{(-1)^k+e^{-\lambda_1 d_{k-1}}[(-1)^{k-1}+\cdots+e^{-\lambda_1 d_3}(-1+e^{-\lambda_1 d_2})\cdots]\}, \quad (A34)$$

$$c_{4,k}^{(k)}=\omega_2 e^{-\lambda_2 d_k}\{(-1)^k+e^{-\lambda_2 d_{k-1}}[(-1)^{k-1}+\cdots+e^{-\lambda_2 d_3}(-1+e^{-\lambda_2 d_2})\cdots]\}. \quad (A35)$$

Note that Eqs. (A32), (A33), (A34), and (A35) do not include d_1. This is a consequence of the translational invariance of Eq. (A5). In fact, d_1 is an arbitrary variable that may be chosen to be zero or some other value dictated by considerations of convenience.

(4) Consider some particular types of solutions to the problem (A5),(A6).

(i) Let us find solutions with $n=1$, i.e., such that the function y changes its sign only once. We have from Eqs. (A10), (A25), (A26) and (A31):

$$y_{1,1}(0)=c_{0,1}^{(1)}+c_{1,1}^{(1)}+c_{2,1}^{(1)}=-(A_1+A_2)/B_0-\omega_1-\omega_2=0.$$

Substituting ω_i from Eq. (A21) and noting an identity

$$\Lambda_1+\Lambda_2=1, \quad (A36)$$

we find that the following identity must hold:

$$A_2=0. \quad (A37)$$

Therefore, a such solution may exist if only Eqs. (A8) and (A37) are true. Then it follows from Eq. (A8) that $y_0=-A_1/B_0$. If this is the case then the solution for $y_0>0$ has the form

$$y_{1,1}(x_1)=y_0[\Lambda_1(1-e^{-\lambda_1 x_1})+\Lambda_2(1-e^{-\lambda_2 x_1})], \quad x_1\geq 0,$$

$$y_{2,1}(x_1)=-y_0[\Lambda_1(1-e^{\lambda_1 x_1})+\Lambda_2(1-e^{\lambda_2 x_1})], \quad x_1<0,$$

or, in a more general form, an antisymmetric solution is finally obtained:

$$y(x)=y_0\,\mathrm{sgn}(x)[\Lambda_1(1-e^{-\lambda_1|x|})+\Lambda_2(1-e^{-\lambda_2|x|})]. \quad (A38)$$

(ii) Let function $y(x)$ have $n=2$ zeros. We express the coefficients $c_{i,1}^{(1)}$ with help of Eqs. (A32) and (A33) to write down for $y_0>0$,

$$y_{1,1}(0)=-(A_1+A_2)/B_0+\omega_1(-1+e^{-\lambda_1 d_2})+\omega_2(-1+e^{-\lambda_2 d_2})=0.$$

Therefore, for arbitrary y_0 we obtain, using Eq. (A9),

$$r\equiv-\mathrm{sgn}(y_0)\frac{A_2}{A_1}=\Lambda_1 e^{-\lambda_1 d_2}+\Lambda_2 e^{-\lambda_2 d_2}. \quad (A39)$$

Note that, by definition, $d_2>0$. Then, taking into account Eqs. (A7) and (A36), we can see that a solution of the given type exists if only

$$0<r<1. \quad (A40)$$

If Eq. (A40) holds and $|A_2|\ll|A_1|$ and/or $\lambda_1\ll\lambda_2$, then $d_2\approx(\lambda_1)^{-1}\ln|\Lambda_1 A_1/A_2|$.

If $y_0>0$, the solutions $y_{1,1}(x_1)$, $y_{2,2}(x_2)$, $y_{3,2}(x_2)$ may be obtained in the form (A10) and unified to be presented in a symmetrical form,

$$y(z)=\frac{A_1-A_2}{B_0}-\frac{2A_1}{B_0}[\Lambda_1 e^{-\lambda_1 d}\cosh(\lambda_1 z)+\Lambda_2 e^{-\lambda_2 d}\cosh(\lambda_2 z)], \quad |z|\leq d, \quad (A41)$$

$$y(z)=-\frac{A_1+A_2}{B_0}+\frac{2A_1}{B_0}[\Lambda_1\sinh(\lambda_1 d)e^{-\lambda_1|z|}+\Lambda_2\sinh(\lambda_2 d)e^{-\lambda_2|z|}], \quad |z|\geq d, \quad (A42)$$

where $d=d_2/2$ and $z=x_1+d=x_2-d$. With the help of identity (A36) and Eq. (A39) it can be easily shown that both Eqs. (A41) and (A42) yield $y(\pm d)=0$.

Upon simple transformations Eqs. (A41) and (A42) may be generalized to cover the case $y_0<0$ as well:

$$y(z)=-y_0\left\{1-\frac{2}{1-r}[-r+\Lambda_1 e^{-\lambda_1 d}\cosh(\lambda_1 z)+\Lambda_2 e^{-\lambda_2 d}\cosh(\lambda_2 z)]\right\}, \quad |z|\leq d,$$

$$y(z)=y_0\left\{1-\frac{2}{1-r}[\Lambda_1\sinh(\lambda_1 d)e^{-\lambda_1|z|}+\Lambda_2\sinh(\lambda_2 d)e^{-\lambda_2|z|}]\right\}, \quad |z|\geq d.$$

This solution is symmetric. Note that the expressions in curly brackets, as shown above, are always positive.

(iii) Let function $y(x)$ have $n>2$ zeros. We substitute the values of $c_{i,1}^{(1)}$ into expression $y_{1,1}(0)=0$ and take into account Eqs. (A17) and (A21) to obtain

$$r=\Lambda_1 e^{-\lambda_1 d_2}(1+e^{-\lambda_1 d_3}\{-1+e^{-\lambda_1 d_4}[1+\cdots+(-1)^n e^{-\lambda_1 d_n}]\cdots\})+\Lambda_2 e^{-\lambda_2 d_2}(1+e^{-\lambda_2 d_3}\{-1+e^{-\lambda_2 d_4}[1+\cdots+(-1)^n e^{-\lambda_2 d_n}]\cdots\}). \quad (A43)$$

On the other hand, the same way we find from condition $y_{2,2}(0)=0$ that

$$r=\Lambda_1(e^{-\lambda_1 d_2}+e^{-\lambda_1 d_3}\{-1+e^{-\lambda_1 d_4}[1+\cdots +(-1)^n e^{-\lambda_1 d_n}]\ldots\})+\Lambda_2(e^{-\lambda_2 d_2}+e^{-\lambda_2 d_3}\{-1 +e^{-\lambda_2 d_4}[1+\cdots+(-1)^n e^{-\lambda_2 d_n}]\cdots\}). \tag{A44}$$

Let us introduce the functions

$$\mathcal{F}_i(t)=-e^{-\lambda_i t}\{-1+e^{-\lambda_i d_4}[1+\cdots +(-1)^{-n}e^{-\lambda_i d_n}]\cdots\}, \quad i=1,2,$$

and

$$\mathcal{F}(t)=\Lambda_1\mathcal{F}_1(t)+\Lambda_2\mathcal{F}_2(t). \tag{A45}$$

Then the result of comparison of Eqs. (A43) and (A44) after simple transformations may be written down as follows:

$$\mathcal{F}(d_2+d_3)=\mathcal{F}(d_3). \tag{A46}$$

The function $\mathcal{F}(t)$ monotonically decreases from $\mathcal{F}(0)<1$ to zero for $t\to+\infty$. It is easy to see therefore that Eq. (A46) can only hold if $d_2=0$ and/or $d_3\to\infty$. Both of these possibilities contradict our assumption $0<d_k<\infty$ for $1<k\leq n$, $n>2$.

Thus, the problem (A5),(A6) has a unique solution for the number of zeros $n=1$ or $n=2$ and does not have solutions for $n>2$.

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