

Supersonic regimes of motion of a topological soliton

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Supersonic regimes of motion of a topological soliton in a bistable molecular chain with cubic anharmonicity of the site–site interaction are studied for the first time. In the framework of the φ^4 model, it is shown that in a bistable symmetric system, anharmonicity of the site–site interaction leads to the result that a positive topological soliton (kink) has a subsonic continuous spectrum and a supersonic discrete spectrum of velocity values. The topological soliton can have only a finite number of supersonic velocity values for which its motion is not accompanied by the emission of phonons. With increase of the anharmonicity, the number of such values increases. Each supersonic topological soliton is a bound state of several acoustic solitons, the sum of the amplitudes of which coincides with the width of the barrier of the two-well potential. © 1995 American Institute of Physics.

1. INTRODUCTION

The development of modern nonlinear physics has led to the discovery of new elementary mechanisms that determine, at the molecular level, the course of many physical processes in crystals and in other ordered systems. Nowadays the role of acoustic solitons, providing the most effective mechanism of energy transport, is entirely clear. Acoustic solitons have supersonic velocities and do not change the state of the system, this being connected with their zero topological charge.^{1–3} On the other hand, topological solitons, describing the transition of a bistable system from one equilibrium state to another, have nonzero topological charge and describe the maximally effective wave mechanism of such a process.^{3–5}

In the absence of anharmonicity of the site–site interaction, topological solitons of opposite sign possess the same properties: they have a continuous subsonic velocity spectrum. Static interaction of topological solitons of opposite signs reduces to their attraction, but in discrete chains, pinning of solitons can lead to the existence of stable bound states of solitons of opposite sign.⁶ In a thermalized chain with a φ^4 potential, an indirect mutually repulsive interaction of solitons of opposite sign occurs via phonons, and is more long-range than the static interaction.⁷ With the appearance of anharmonicity of the site–site interaction, the situation changes sharply. The properties of topological solitons of opposite sign now become different. Thus, in Ref. 8 it was shown that with increase of negative anharmonicity, the velocity spectrum of a negative soliton is compressed, and when a threshold value is reached, it even disappears (the soliton has only zero velocity), whereas a positive soliton always has a continuous subsonic velocity spectrum. In Ref. 9 it was shown that anharmonicity can lead to the result that a positive topological soliton has one supersonic value of the velocity, but the structure of the supersonic velocity spectrum has remained unclear up to now. The aim of the present paper is to investigate the structure of the supersonic velocity spectrum of a topological positive soliton in the φ^4 model with negative cubic anharmonicity of the site–site interaction.

In this paper we perform a numerical investigation of the supersonic regimes of motion of a positive topological soliton (kink). It will be shown that the supersonic spectrum has a discrete structure. There exist only a finite number of supersonic velocity values $s_1 > s_2 > \dots > s_N$ for which the motion of the kink is not accompanied by the emission of phonons. The supersonic kink corresponding to the n th velocity value s_n is a bound state of n acoustic (nontopological) solitons. For the other supersonic velocity values, the motion of the kink will always be accompanied by the emission of phonons.

2. THE MODEL

The Hamiltonian of the bistable molecular chain has the form

$$\mathcal{H} = \sum_n \left[\frac{1}{2} m \dot{u}_n^2 + \mathcal{U}(u_{n+1} - u_n) + \mathcal{V}(u_n) \right], \quad (1)$$

where m is the mass of a link of the chain, u_n is the displacement of the n th link from its equilibrium position, $\mathcal{U}(\rho)$ is the site–site interaction potential, and $\mathcal{V}(u)$ is the symmetric two-well potential describing the interaction of the sites of the chain with its substrate. For the φ^4 model with cubic anharmonicity,

$$\mathcal{U}(\rho) = \frac{1}{2} \kappa \rho^2 - \frac{1}{3} \gamma \rho^3, \quad \mathcal{V}(u) = \varepsilon \left[\left(\frac{u}{l} \right)^2 - 1 \right]^2,$$

where κ and $\gamma > 0$ are the stiffness and anharmonicity of the site–site interaction, and ε and $2l$ are the height and width of the barrier of the two-well potential.

Corresponding to the Hamiltonian (1) is the following system of equations of motion:

$$m \ddot{u}_n = \mathcal{F}(u_{n+1} - u_n) - \mathcal{F}(u_n - u_{n-1}) - \mathcal{G}(u_n), \quad (2)$$
$$n = 0, \pm 1, \pm 2, \dots,$$

where

$$\mathcal{F}(\rho) = \frac{d}{d\rho} \mathcal{H}(\rho) = \kappa\rho - \gamma\rho^2, \quad \mathcal{G}(u) = \frac{d}{du} \mathcal{Z}(u) = 4\epsilon u((u/l)^2 - 1)/l^2.$$

For convenience we introduce the dimensionless time $\tau = t\sqrt{\kappa/m}$, dimensionless displacements $x_n = u_n/l$, and dimensionless energy $H = \mathcal{H}/\kappa l^2$. Then the Hamiltonian (1) of the system will have the form

$$H = \sum_n \left\{ \frac{1}{2} x_n'^2 + U(r_n) + V(x_n) \right\}, \quad (3)$$

where the prime denotes differentiation with respect to the dimensionless time τ , $r_n = x_{n+1} - x_n$ are the relative displacements, and

$$U(r) = \frac{1}{2} r^2 - \frac{1}{3} \beta r^3, \quad V(x) = g(x^2 - 1)^2,$$

in which $\beta = \gamma l/\kappa > 0$ is the dimensionless anharmonicity parameter and $g = \epsilon/\kappa l^2 \geq 0$ is the dimensionless height of the barrier of the two-well potential. The equations of motion (2) take the form

$$x_n'' = F(r_n) - F(r_{n-1}) - G(x_n), \quad n = 0, \pm 1, \pm 2, \dots, \quad (4)$$

where

$$F(r) = \frac{d}{dr} U(r) = r - \beta r^2, \quad G(x) = \frac{d}{dx} V(x) = 4gx(x^2 - 1).$$

3. THE CONTINUUM APPROXIMATION

We shall assume that the system of differential equations (4) has a soliton solution $x_n(\tau) = x(\xi) = x(n - st)$ that depends smoothly on the label n of the chain site, i.e., a solution in the form of a solitary wave of constant shape with the asymptotic form

$$x_n \rightarrow \mp 1 (\pm 1) \quad \text{as } n \rightarrow \pm \infty \quad (5)$$

for a positive (negative) soliton. Here, $\xi = n - st$ is the wave variable and s is the soliton velocity. A positive topological soliton describes the transition of the chain from the equilibrium state $x_n \equiv +1$ to the other equilibrium state $x_n \equiv -1$, while a negative topological soliton describes the reverse transition. In the region of localization of a positive soliton compression of the chain occurs, while in the region of localization of a negative soliton extension of the chain occurs.

Without allowance for dispersion of long-wavelength phonons, the system of equations of motion (4) in the continuum approximation reduces to the differential equation

$$(1 - s^2)x_{\xi\xi} - 2\beta x_{\xi}x_{\xi\xi} - 4gx(x^2 - 1) = 0. \quad (6)$$

This equation can be integrated, making it possible in this approximation to investigate completely the properties of topological solitons in an anharmonic chain.⁹

In fact, letting $\varphi = x_{\xi}$, Eq. (6) takes the form

$$[1 - s^2 - 2\beta\varphi]d\varphi = 4gx(x^2 - 1)d\xi. \quad (7)$$

We multiply Eq. (7) by φ , and then integrate it, taking into account the boundary conditions (5). We obtain

$$\left[\frac{1}{2} (1 - s^2) - \frac{2}{3} \beta \varphi \right] \varphi^2 = g(x^2 - 1)^2. \quad (8)$$

For a positive soliton ($\varphi \leq 0$) we can obtain from Eq. (8) a continuous dependence $\varphi = \varphi(x)$ ($-1 \leq x \leq 1$) only if $|s| \leq 1$, while for a negative soliton ($\varphi \geq 0$) we can obtain from Eq. (8) a continuous dependence $\varphi = \varphi(x)$ ($-1 \leq x \leq 1$) only if $|s| < s_-$, where

$$s_- = \sqrt{1 - (24\beta^2 g)^{1/3}} \quad \text{for } 24\beta^2 g \leq 1,$$

$$s_- = 0 \quad \text{for } 24\beta^2 g > 1.$$

Thus, the use of the continuum approximation without allowance for the dispersion of long-wavelength phonons shows that a positive topological soliton always has only a continuous subsonic spectrum of velocities $0 \leq s \leq 1$, while a negative topological soliton always has only a continuous spectrum $0 \leq s \leq s_-$.

When the dispersion of the long-wavelength phonons is taken into account, the equations of motion (4) in the continuum approximation now reduce to

$$(1 - s^2)x_{\xi\xi\xi} + \frac{1}{12}x_{\xi\xi\xi\xi\xi} - 2\beta x_{\xi}x_{\xi\xi\xi} - 4gx(x^2 - 1) = 0, \quad (9)$$

which, in the general case, cannot be integrated analytically.

In Ref. 8 it is shown that Eq. (9) for a fixed velocity

$$s = s'_1(\beta) = \sqrt{1 + \frac{4}{3}\beta^2 - \frac{1}{2\beta^2}g} \quad (10)$$

has a soliton solution

$$x(\xi) = -\tanh(\mu\xi/2) \quad (11)$$

with inverse width $\mu = 4\beta$. It follows from Eq. (10) that for a small height g of the barrier of the two-well potential, the positive topological soliton (11) has a supersonic velocity $s = s'_1(\beta) > 1$.

In the limit $g \rightarrow 0$, Eq. (9), after one integration, goes over into the Boussinesq equation

$$\frac{1}{12}\varphi_{\xi\xi\xi} + (1 - s^2)\varphi - \beta\varphi^2 = 0,$$

which yields the supersonic acoustic soliton

$$\varphi(\xi) = -a/\cosh^2(\mu\xi)$$

in a one-dimensional lattice with cubic anharmonicity; here, $a = 3(s^2 - 1)/2\beta$, the inverse width $\mu = \sqrt{3(s^2 - 1)}$, and the velocity $s > 1$. The boundary condition (5), which is preserved in the limit $g \rightarrow 0$, makes only one velocity value allowed for the acoustic phonon:

$$s = \sqrt{1 + \frac{4}{3}\beta^2}. \quad (12)$$

In fact, the total chain compression, which henceforth we shall call the amplitude of the acoustic soliton, is

$$R(s) = x(+\infty) - x(-\infty) = \int_{-\infty}^{+\infty} \varphi(\xi) d\xi = -\sqrt{3(s^2 - 1)}/\beta = -2,$$

which follows Eq. (12). We note also that Eq. (12) is obtained from (10) in the limit $g \rightarrow 0$.

On the other hand, for $g=0$ the boundary condition (5) will also be fulfilled when several identical acoustic solitons are present in the system. In this case the velocity s_N of the N -soliton state can be found from the equation $NR(s_N) = -2$, and is equal to

$$s_N^0(\beta) = \sqrt{1 + \frac{4}{3} (\beta/N)^2}. \quad (13)$$

Thus, in the limit $g \rightarrow 0$, a positive topological soliton has an infinite discrete supersonic spectrum $\{s_N^0\}_{N=1}^\infty$, with the sound velocity $s=1$ as the limit point. It is not possible to find the N -soliton solution of Eq. (9) analytically for $N \geq 2$ and $g > 0$, and so we shall seek it numerically.

4. NUMERICAL DETERMINATION OF THE SUPERSONIC STATES OF A TOPOLOGICAL SOLITON

Again we shall assume that the equations of motion (4) of the chain have a solution $x_n(\tau) = x(n - s\tau)$ that depends smoothly on n and satisfies the asymptotic form (5). Then, if we replace the second time derivative by its discrete analog

$$x_n'' = s^2 \frac{d^2}{dn^2} x = \frac{1}{12s^2} [16(x_{n+1} - 2x_n + x_{n-1}) - (x_{n+2} - 2x_n + x_{n-2})],$$

the system of differential equations (4) is transformed into a system of purely discrete equations

$$-\frac{1}{12} s^2 [16(x_{n+1} - 2x_n + x_{n-1}) - (x_{n+2} - 2x_n + x_{n-2})] + F(r_n) - F(r_{n-1}) - G(x_n) = 0, \quad (14)$$

$$n = 0, \pm 1, \pm 2, \dots,$$

which in the continuum approximation coincides with Eq. (9).

The system of discrete equations (14) determines an extremum of the Lagrangian

$$L_s = \sum_n \left\{ -\frac{1}{24} s^2 [16(x_{n+1} - x_n)^2 + (x_{n+2} - x_n)^2] + U(x_{n+1} - x_n) + V(x_n) \right\}.$$

Therefore, the soliton solutions of Eq. (9) can be sought numerically as extrema of the Lagrangian L_s . A supersonic topological soliton corresponds to a saddle point of the Lagrangian, and, therefore, it can be found by solving the problem numerically for a conditional minimum:

$$F_s = \frac{1}{2} \sum_{n=3}^{M-2} \left(\frac{\partial L_s}{\partial x_n} \right)^2 \rightarrow \min_{x_3, \dots, x_{M-2}} : x_1 = x_2 = +1, \quad (15)$$

$$x_{M-1} = x_M = -1.$$

The boundary conditions should have no effect on the shape of the soliton; for this it is sufficient to take the number M of sites to be ten times the width of the soliton.

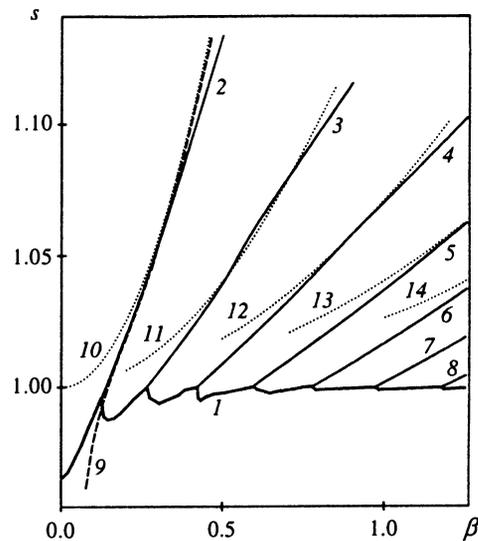


FIG. 1. Dependence of the upper boundary s_0 of the continuous spectrum of velocity values (thick curve 1), the supersonic values s_1, s_2, \dots, s_7 (thin curves 2, 3, ..., 8), s_1^0 (dashed curve 9), and $s_1^0, s_2^0, \dots, s_5^0$ (dotted curves 10, 11, ..., 14) on the anharmonicity parameter β of the chain.

In solving the minimum problem (15) numerically we used the method of conjugate gradients, and took $M=400$. The solution of this problem makes it possible to find all the soliton solutions of Eq. (9). The minimum point $\{x_n^0\}_{n=1}^M$ of the functional F_s corresponds to a soliton solution only if x_n^0 depends smoothly on n , and the actual minimum value $F_s(x_1^0, \dots, x_M^0) \approx 0$. If the functional F_s has no such minima, this indicates unambiguously that Eq. (14), and hence Eq. (9), does not have soliton solutions for the velocity value s used.

5. SUPERSONIC STATES OF A TOPOLOGICAL SOLITON

For definiteness we shall take for the substrate parameter one specific value ($g=0.001$). Numerical solution of the minimum problem (15) showed that a positive topological soliton always has a continuous subsonic velocity spectrum $0 \leq s \leq s_0 \leq 1$. The dependence of the upper boundary s_0 of the continuous spectrum on the anharmonicity parameter β is given in Fig. 1. For $\beta=0$ we have $s_0=0.966$, and as the anharmonicity increases, the upper boundary of the continuous spectrum tends to the velocity of sound: $s_0 \rightarrow 1$ as $\beta \rightarrow \infty$.

In addition to the continuous subsonic spectrum, the soliton has a finite discrete supersonic velocity spectrum $\{s = s_n\}_{n=1}^N$, where $s_1 > \dots > s_N > 1$ (for other values of $s > 1$, the problem (15) does not have soliton solutions). The number N of accessible supersonic values of the velocity increases monotonically as the anharmonicity parameter β increases. There exists a sequence (tending to infinity) of values of β

$$0 < \beta_1 < \beta_2 < \dots < \beta_n < \dots,$$

at which the number N increases by unity. Thus, for $0 \leq \beta < \beta_1$ we have $N=0$ (the topological soliton does not have supersonic states), and for $\beta_n \leq \beta < \beta_{n+1}$ we have

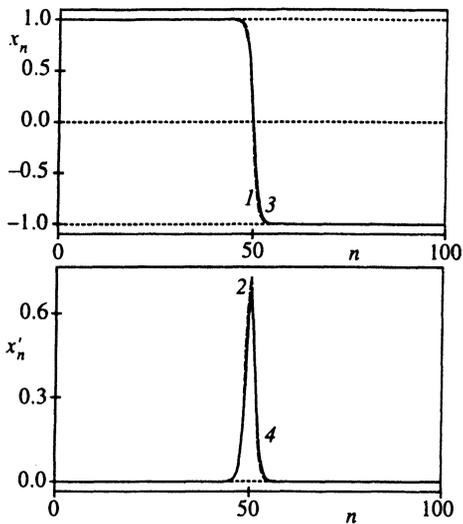


FIG. 2. Form of the one-soliton supersonic kink state found by numerical solution of the problem (15), at the initial time $\tau=0$ (dashed curves 1 and 2) and at the time $\tau=\tau_e=92542.1$ after $N=100000$ links have been passed (solid curves 3 and 4). The anharmonicity parameter $\beta=0.4$, the barrier height $g=0.001$, the initial velocity $s_1=1.095$, and the final velocity $\bar{s}_1=1.079$.

$N=n$ (the topological soliton has $n=1, 2, \dots$ supersonic states). For the parameter value $g=0.001$ used here the critical values of the anharmonicity parameter are $\beta_1=0.12$, $\beta_2=0.25$, $\beta_3=0.42$, $\beta_4=0.59$, $\beta_5=0.78$, $\beta_6=0.97$, $\beta_7=1.17$.

The supersonic velocities s_n increase monotonically with increasing anharmonicity parameter. In Fig. 1 we show the dependence on β of the supersonic values s_1, s_2, \dots, s_7 . As can be seen from the figure, the dependence $s_1(\beta)$ obtained by numerical solution of the problem (15) is essentially identical with the dependence $s'_1(\beta)$ obtained analytically. The corresponding curves 2 and 9 in Fig. 1 differ only at velocities $s > 1.07$, when the soliton becomes narrow and the continuum approximation that we have used ceases to be correct.

From Fig. 1 it can be seen that as $\beta \rightarrow \infty$, the functions $s_n(\beta)$ and $s_n^0(\beta)$ behave equivalently [$s_n(\beta)/s_n^0(\beta) \rightarrow 1$]. In the limit, the supersonic topological-soliton (kink) state that has velocity s_n decays into n identical acoustic solitons, and therefore we shall call such a state an n -soliton state. From this we can also conclude that the discreteness of the supersonic velocity spectrum is due entirely to the presence of the boundary condition (5), i.e., to the two-well nature of the potential $V(x)$, and not to its specific form.

In Fig. 2 we give a characteristic graph of a one-soliton supersonic kink state. From the relative displacements $r_n = x_{n+1} - x_n$ of the links of the chain, which are proportional to the velocities x'_n ($x'_n \approx -sr_n$), the kink has a one-hump profile. The one-soliton state can be considered to be an acoustic soliton satisfying the boundary condition (5). In Figs. 3, 4, and 5 we give characteristic graphs for two-, three-, and four-soliton supersonic kink states. The corresponding kinks have two-, three-, and four-hump profiles in the relative displacements. This shows that the given supersonic states are bound states of two, three, and four acoustic

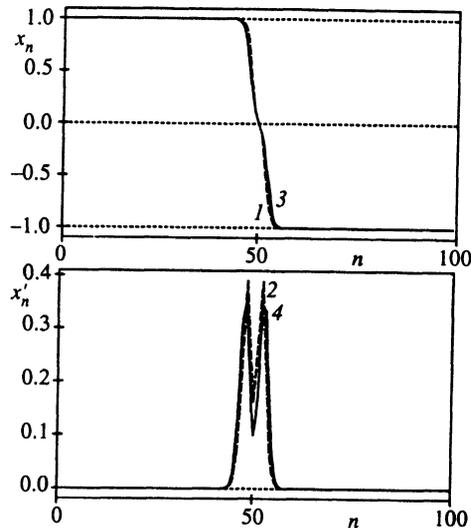


FIG. 3. Form of the two-soliton supersonic kink state. All the notation coincides with that of Fig. 2; $\beta=0.9$, $g=0.001$, $s_2=1.115$, $\bar{s}_2=1.095$, $N=50000$, $\tau_e=45530.0$.

solitons. In the next section, it will be shown that if we take away the substrate, i.e., take $g=0$, the n -soliton state decays into n acoustic solitons.

6. NUMERICAL MODELING OF THE DYNAMICS OF SUPERSONIC STATES OF A TOPOLOGICAL SOLITON

We consider the dynamics of the supersonic states obtained for a topological soliton (kink) in a finite chain of L kinks with free ends. The dynamics of such a chain is specified by the equations of motion

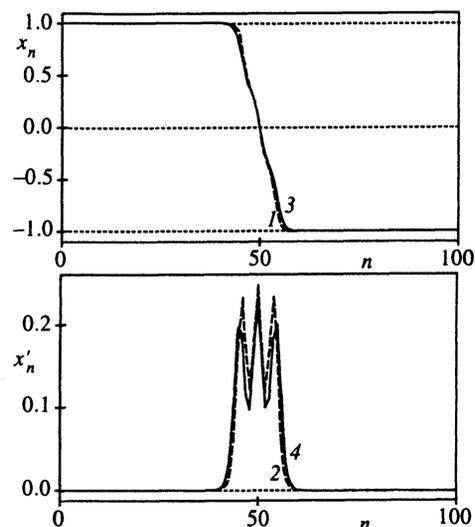


FIG. 4. Form of the three-soliton supersonic kink state. All the notation coincides with that of Fig. 2; $\beta=1.1$, $g=0.001$, $s_3=1.083$, $\bar{s}_4=1.065$, $N=50000$, $\tau_e=46823.0$.

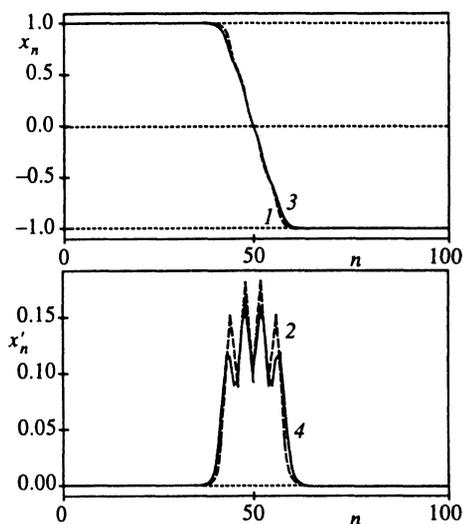


FIG. 5. Form of the four-soliton supersonic kink state. All the notation coincides with that of Fig. 2; $\beta=1.2$, $g=0.001$, $s_4=1.058$, $\bar{s}_4=1.041$, $N=50,000$, $\tau_e=47944.8$.

$$\begin{aligned}
 x_1'' &= F(r_1) - G(x_1), \\
 &\dots \\
 x_n'' &= F(r_n) - F(r_{n-1}) - G(x_n), \\
 &\dots \\
 x_L'' &= -F(r_{L-1}) - G(x_L)
 \end{aligned}
 \tag{16}$$

with the energy integral

$$H = \sum_{n=1}^L \left[\frac{1}{2} x_n'^2 + V(x_n) \right] + \sum_{n=1}^{L-1} U(r_n).
 \tag{17}$$

The number L of sites in the chain will be taken to be equal to $M+100$, where M is the number of sites used in the solution of the minimum problem (15). To the soliton solution $\{x_n^0\}_{n=1}^M$ (with velocity s) of the problem (15) corresponds the initial condition

$$\begin{aligned}
 x_n(0) &= x_n^0, \quad \text{for } n=1, 2, \dots, M, \\
 x_n(0) &= x_M^0, \quad \text{for } n=M+1, \dots, L, \\
 x_n'(0) &= -s(x_{n+1}(0) - x_{n-1}(0))/2, \\
 &\text{for } n=2, \dots, L-1, \\
 x_1'(0) &= 0, \quad x_L'(0) = 0.
 \end{aligned}
 \tag{18}$$

The center of the soliton $\{x_n(\tau)\}_{n=1}^L$ is conveniently defined as the point at which the broken line sequentially linking the points (n, x_n) intersects the n axis. At the initial time the soliton has center $m=M/2$. In order to model the dynamics of the soliton in an infinite chain, each time it passes through 100 links of the chain, i.e., each time its center reaches the site $M/2+100$, we shift the soliton to the left through 100 links, i.e., make the replacement

$$x_n = x_{100+n}, \quad x_n' = x'_{100+n}, \quad \text{for } n=1, \dots, M,$$

$$x_n = x_L, \quad x_n' = 0, \quad \text{for } n=M+1, \dots, L.$$

This method of numerical modeling of the dynamics of a topological soliton makes it possible to avoid integration of a system of high dimensionality. It is especially convenient for analysis of the dynamics of supersonic solitons. With each shift the nonsoliton subsonic component of the initial condition is cut off.

Numerical modeling of the dynamics of a topological soliton confirmed the discreteness of the supersonic spectrum of velocity values. As can be seen from Figs. 2–5, starting with the initial condition (18) corresponding to an n -soliton supersonic ($s=s_n>1$) kink state, a supersonic kink of constant shape, moving along the discrete chain with a constant supersonic velocity $s=\bar{s}_n<s_n$, is formed.

The initial condition (18), obtained using the continuum approximation, is not exact for a soliton on a discrete chain. The discreteness of the chain causes the actual velocity value \bar{s}_n to differ from the calculated value s_n . The motion of a supersonic kink is always accompanied by the emission of phonons, as long as the kink velocity $s>\bar{s}_n$. The emission of phonons leads to slowing down of the kink. At the velocity $s=\bar{s}_n$ the emission disappears, and the motion of the kink is completely stabilized. The kink now begins to move with this constant velocity, and its shape does not change. We note that the final velocity $s=\bar{s}_n$ does not change with small variations in the initial velocity and shape of the kink. Such stability is an unambiguous indication that the supersonic velocity spectrum of a kink in an anharmonic chain is discrete.

In order to understand the structure of a supersonic state of a kink, we consider the dynamics of a kink in a chain without a substrate ($g=0$). For this we integrate the equations of motion (16) for $g=0$ and $L=1100$. We shall take the initial condition corresponding to a supersonic n -soliton ($n=1, \dots, 5$) state of a kink in a discrete chain with a substrate ($g=0.001$). The integration showed that, in this case, exactly n uncoupled acoustic solitons and a subsonic phonon tail are formed from the kink (see Fig. 6). This makes it possible to conclude that the supersonic n -soliton state of the kink is indeed a bound state of n acoustic solitons that is stable at only one velocity value $s=\bar{s}_n$.

The dependence of the velocity \bar{s}_n of the n -soliton supersonic state of a kink in a discrete chain on the anharmonicity parameter β is shown in Fig. 7. The value of the velocity \bar{s}_n agrees well with the calculated value of s_n only near the sound velocity. In this case the large kink width makes the continuum approximation used in the preceding section appropriate. Despite this, the numerical modeling performed for the supersonic dynamics of the kink suggests that the result that the supersonic spectrum of velocity values is discrete remains true for higher velocity values as well, when the kink width becomes commensurate with the chain step. Here, however, the derivation of an accurate value for the velocity requires the use of more involved methods that take the discreteness of the chain into account.¹⁰

At a subsonic velocity $s<1$, a positive topological soliton has a large width, and therefore solving the minimum

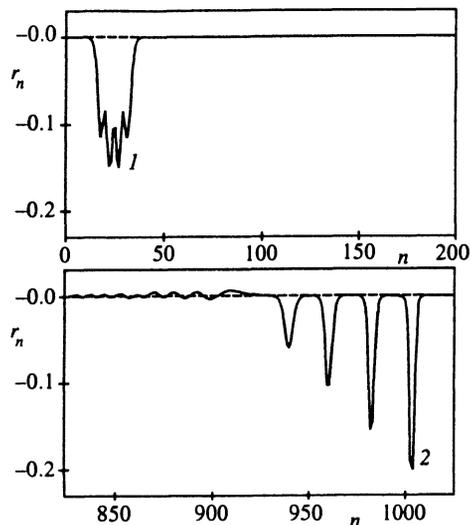


FIG. 6. Decay of the four-soliton supersonic kink state ($\beta=1.2$, $g=0.001$, $\bar{s}_4=1.041$) on a free chain ($g=0$) into four acoustic solitons and a subsonic phonon tail. Curve 1 shows the relative displacements $r_n=x_{n+1}-x_n$ of the links of the chain at the initial time $\tau=0$, and curve 2 shows the same at time $\tau=900$. The chain length $L=1100$.

problem (15) makes it possible to find the shape of the soliton with high accuracy; see Fig. 8.

The numerical integration of the equations of motion (16) was performed by the standard Runge-Kutta method with fourth-order accuracy and a constant integration step. The accuracy of the numerical integration was checked using constancy of the energy integral (17). With the step value used ($\Delta\tau=0.05$), the energy remained constant to five significant figures.

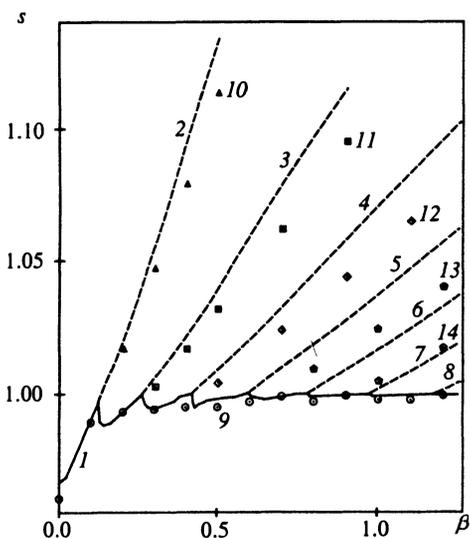


FIG. 7. Dependence of the velocity values s_0, s_1, \dots, s_7 on the anharmonicity parameter β (curves 1, 2, ..., 8). The markers 9, 10, ..., 14 give the velocity values $\bar{s}_0, \bar{s}_1, \dots, \bar{s}_5$ obtained by numerical modeling of the soliton dynamics.

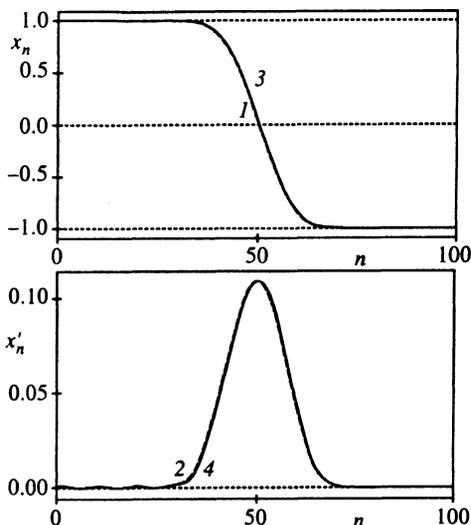


FIG. 8. Form of a subsonic topological soliton at the initial time $\tau=0$ (dashed curves 1 and 2) and at the time $\tau=10103.0$ after $N=10000$ links of the chain have been passed (solid curves 3 and 4). The initial velocity $s=0.99$, $\beta=1.0$, $g=0.001$, and the velocity $\bar{s}=0.9898$.

7. CONCLUSION

In this paper it has been shown for the first time that in a bistable molecular chain with cubic anharmonicity of the site-site interaction, a topological soliton (kink) has a finite discrete supersonic spectrum of velocity values. There exist only a finite number of velocity values $s_1 > s_2 > \dots > s_N > 1$ for which the motion of the soliton is not accompanied by the emission of phonons. A supersonic kink corresponding to the n th velocity value s_n is a bound state of n acoustic solitons, the sum of the amplitudes of which should coincide with the width of the barrier of the two-well potential. The number N of supersonic velocity values increases with increasing anharmonicity parameter of the chain. In the framework of the continuum approximation we have proposed a numerical method of determination of the shape and velocity of the supersonic states of a topological soliton.

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