Stability of spatial structures and annihilation of soliton–antisoliton pairs in a discrete φ^4 model

V. V. Beloshapkin, G. P. Berman, and A. G. Tretyakov

L. V. Kirenski Institute of Physics, Siberian Branch of the Academy of Sciences of the USSR, Krasnoyarsk

(Submitted 24 July 1988)
Zh. Eksp. Teor. Fiz. **95**, 723–731 (February 1989)

An analysis is made of the stability of soliton configurations using a discrete φ^4 model. It is shown that destruction of equilibrium structures represents soliton–antisoliton pair annihilation in the absence of a phason mode in a spectrum of small vibrations. The role of temperature and quantum fluctuations is investigated.

Considerable progress has been made recently in the study of structure states deduced using discrete nonlinear one-dimensional models. For example, the Frenkel–Kontorova (FK) discrete model has been investigated sufficiently thoroughly. Detailed reviews can be found in Refs. 1 and 2. In particular, it has been shown that in a certain range of parameters the discrete effects can result in pinning of regular soliton configurations and can also give rise to stochastic structure states. For example, Peyrard and Aubry[3] investigated numerically the characteristics of a one-dimensional model of atoms in a periodic potential such as the gap in the phonon spectrum, the coherence length, the Peierls–Nabarro barrier, and the pinning force in the vicinity of a transition corresponding to a discontinuity of analyticity. It was shown in Ref. 3 that there is a critical value of the amplitude of a periodic external field λ_c in which a periodic soliton structure is pinned and the spectrum of small vibrations exhibits a gap Δ:

$$\Delta(\lambda)\sim(\lambda-\lambda_c)^x, \qquad x\sim 1.$$

If $\lambda<\lambda_c$, a soliton structure is not pinned and can glide freely along a chain. A phason mode then appears in the spectrum of the frequency of atomic vibrations. The transition from pinning to depinning was considered in Refs. 4 and 5 in describing a metal–insulator transition in Peierls chains.

We consider some properties of a discrete φ^4 model used widely in the description of structural transitions in ferroelectrics, proton transport processes in quasi-one-dimensional chains with hydrogen bonds,[6] etc.

We show numerically that in a discrete chain of harmonically coupled particles, which are in a two-well potential, the attraction between solitons and antisolitons is exponential. This interaction has the effect that for any density of solitons there is such a critical value of the parameter of the one-particle potential K_{cr} above which the state of a system with a given soliton density is dynamically stable, whereas in the range $K<K_{cr}$ we can expect annihilation of soliton–antisoliton pairs resulting in the appearance either of a homogeneous state or of a structure with one soliton.

We show that the spectrum of small vibrations of atoms in a soliton configuration chain does not contain a phason mode in a wide range of the parameter K. This demonstrates the absence of unpinned soliton structures in the discrete φ^4 model, in contrast to the FK discrete model.[1,3]

We report an investigation of the influence of temperature and quantum fluctuations on the structure states predicted by this model using the approximation of a self-consistent phonon field. We shall show that temperature and quantum fluctuations lower the threshold for the annihilation of soliton–antisoliton pairs.

The Hamiltonian of this model is

$$H=\sum_n \frac{p_n^2}{2m}+\frac{\gamma}{2}\sum_n (u_{n+1}-u_n)^2+V_0\sum_n\left(\frac{u_n^2}{b^2}-1\right)^2, \tag{1}$$

where p_n and u_n are the momentum and displacement of the nth atom measured from the center of a two-well potential; γ is the elastic constant of the chain; V_0 and $2b$ are the energy barrier and the distance between the two wells of a one-particle potential. Introducing a dimensionless variable $\varphi_n=u_n/b$, as well as the parameters $\omega_0^2=\gamma/m$ and $K=V_0/\gamma b^2$, we shall consider the following Hamiltonian:

$$\mathcal{H}=\frac{H}{\gamma b^2}=\frac{1}{2\omega_0^2}\sum_n \dot{\varphi}_n^2+\frac{1}{2}\sum_n(\varphi_{n+1}-\varphi_n)^2 +K\sum_n(\varphi_n^2-1)^2. \tag{2}$$

Steady-state equilibrium states of a chain are described by the following equations:

$$\frac{\partial\mathcal{H}}{\partial\varphi_n}=-\varphi_{n+1}+2\varphi_n-\varphi_{n-1}+4K\varphi_n(\varphi_n^2-1)=0, \tag{3}$$

which can be written in the form of a discrete mapping

$$I_{n+1}=I_n+4K\varphi_n(\varphi_n^2-1), \quad \varphi_{n+1}=\varphi_n+I_{n+1}. \tag{3a}$$

The ground state of the model described by Eq. (2) is doubly degenerate and corresponds to the position of the particles either in the wells on the right-hand side ($\varphi_n=1$) or in the wells on the left-hand side ($\varphi_n=-1$). In the simplest case, solitons are related to a transition of some of the particles from the state $\varphi=1$ to the state $\varphi=-1$. An antisoliton corresponds to a transition $\varphi_n=-1\to\varphi_n=1$. A special feature of the φ^4 model is that solitons and antisolitons alternate rigorously along a chain. In particular, this is one of the differences between the φ^4 and the FK models, because in the latter case the alternation of compression and dilatation solitons is not essential and, moreover, the structure of the ground state obtained in the FK model always includes either solitons or antisolitons.

We investigate dynamically stable equilibrium configurations of the model of Eq. (2) by the gradient method.[3,7–9] In this method we solve a system of equations

$$\dot{\varphi}_n=-\partial\mathcal{H}/\partial\varphi_n, \qquad n=1-N. \tag{4}$$

 0038-5646/89/020410-05$04.00

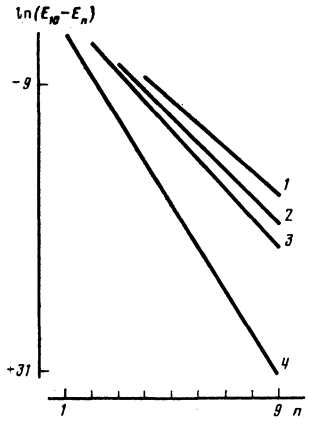

FIG. 1. Dependence of the energy of a chain E_n on the distance between a soliton and an antisoliton for different values of K: 1) 0 5; 2) 0.7; 3) 0.9; 4) 3.

If $t \to \infty$, all the quantities $\{\varphi_n\}$ tend to the values at which the investigated system has a stable equilibrium position.

The first step is the interaction of a soliton and an antisoliton. We considered this step for a chain of 30 particles. We selected the initial conditions in integration of the system of equations (4) so that one soliton and one antisoliton should form in the chain. Variation of the distance between the centers of the soliton and antisoliton was used in calculating the energy of the chain. The results of this calculation are plotted in Fig. 1 for different values of the parameter K. The ordinate gives the quantity $\ln(E_{10} - E_n)$, where E_{10} is the energy of a chain in which the distance between solitons and antisolitons is equal to 10 chain periods. Such a selection of the origin for the measurement of the energy is made because in the range $n > 10$ a change in n by unity changes the energy in the 14th or 15th decimal place, which is at the limit of the precision attainable on a computer. It is clear from Fig. 1 that the energy of interaction of such a soliton and an antisoliton decreases exponentially as the distance between them is reduced, which is in agreement with the results obtained in the continuum approximation.[10,11] Next, as we can see from Fig. 1, a soliton and an antisoliton can approach only to a certain finite distance. For a fixed value of K their approach to a distance less than a certain critical value results in mutual annihilation and the system goes over to a homogeneous state. In reality, such a transition releases an

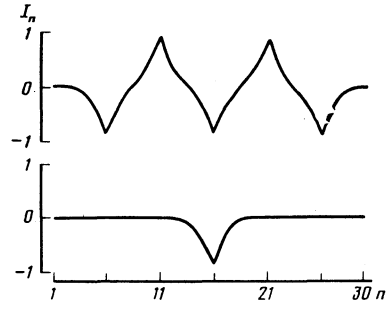

FIG. 2. Regular soliton structure in a chain of 30 particles. The upper part of the figure shows a soliton structure above the annihilation threshold of a pair in the case when $K = 0.3250$. The lower part of the figure shows a structure after annihilation for $K = 0.2999$.

FIG. 3. The gap in the spectrum of small vibrations of a structure shown in the upper part of Fig. 1 as a function of the parameter K in the vicinity of the soliton–antisoliton annihilation threshold.

energy which is used to create dynamic excitations of the phonon type, which is discussed later.

The opposite is also true, i.e., a reduction in the parameter K for a fixed distance n between the centers of a soliton and an antisoliton to a value K_{cr} (which depends on n) results in the annihilation of the soliton–antisoliton pair. If $K > K_{cr}$, both the soliton and antisoliton are pinned and the force of attraction between them is compensated by the force of pinning to the lattice. In particular, this means that a reduction in the parameter K reduces the pinning force faster than the attraction force. Naturally, for a regular soliton lattice (i.e., a regular sequence of solitons and antisolitons) there should be a critical value K_{cr} below which the mutual annihilation of solitons and antisolitons takes place. An example of such a transition is shown in Fig. 2. We started with an initial structure of a chain consisting of 30 particles and containing two solitons and three antisolitons in the case when $K = 0.325$ (upper part of Fig. 2). The lower part of the same figure shows the structure of the same chain when K is reduced to $K = 0.299$, i.e., after the annihilation of two solitons and two antisolitons. We then investigated the behavior of the gap in the spectrum of small vibrations of particles in a soliton equilibrium configuration in the vicinity of the annihilation threshold. The gap in the vibration spectrum was defined as the smallest eigenvalue of the system

$$|\mathcal{H}_{nn'} - \omega^2 \delta_{nn'}| = 0, \qquad \mathcal{H}_{nn'} = \partial^2 \mathcal{H} / \partial \varphi_n \partial \varphi_{n'}. \tag{5}$$

Figure 3 shows the dependence of the lowest frequency in the spectrum of vibrations described by Eq. (5), representing a chain with the Hamiltonian of Eq. (2); this lowest frequency is plotted as a function of the parameter K of the one-particle potential. As a stable equilibrium structure we

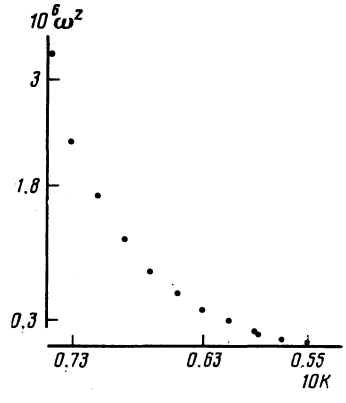

FIG. 4. The gap in the spectrum of small vibrations of a one-soliton structure as a function of the parameter K for a chain of 50 particles.

used that shown in Fig. 2. We can see that in the vicinity of a transition ($K_{cr} \sim 0.3$) the lowest frequency ω_{min} exhibits considerable softening. However, this frequency does not vanish completely (if we allow for the calculation error).

We investigated the pinning conditions in a one-soliton structure by finding how the gap in the spectrum of small vibrations of a chain consisting of 50 particles depends on the parameter K (Fig. 4). On the basis of this dependence we concluded that a one-soliton configuration in the discrete φ^4 model is pinned when K is reduced to values of $\sim 10^{-7}$. On further reduction in K the width of a soliton becomes so large that it is necessary to select very long chains simply in order to avoid the influence of the boundary conditions.

We shall now consider the problem of evolution of an equilibrium structure subject to allowance for dynamic excitations of a chain. We studied this evolution by numerical analysis of the solutions of the equations of motion of atoms in a chain containing $N = 250$ particles, subject to the following cyclic boundary conditions:

$$\dot{p}_n = -\partial\mathcal{H}/\partial\varphi_n, \quad \dot{\varphi}_n = \partial\mathcal{H}/\partial p_n, \qquad \varphi_{N+1} = \varphi_1, \quad n = 1-N. \tag{6}$$

The initial conditions were selected in the form of a stable regular soliton structure consisting of two soliton–antisoliton pairs. We assumed that all the solitons have a finite velocity sufficient to overcome the pinning barrier. This velocity corresponds to the following initial velocities of the atoms in a chain:

$$\dot{\varphi}_n(t=0) = -v\left.\frac{\partial\varphi_n}{\partial x_n}\right|_{t=0}. \tag{7}$$

Figure 5 shows the instantaneous configurations of this chain at various moments. We can see that initially a soliton structure moves as a whole at a velocity v. Next, the influence of attraction between solitons and antisolitons results in

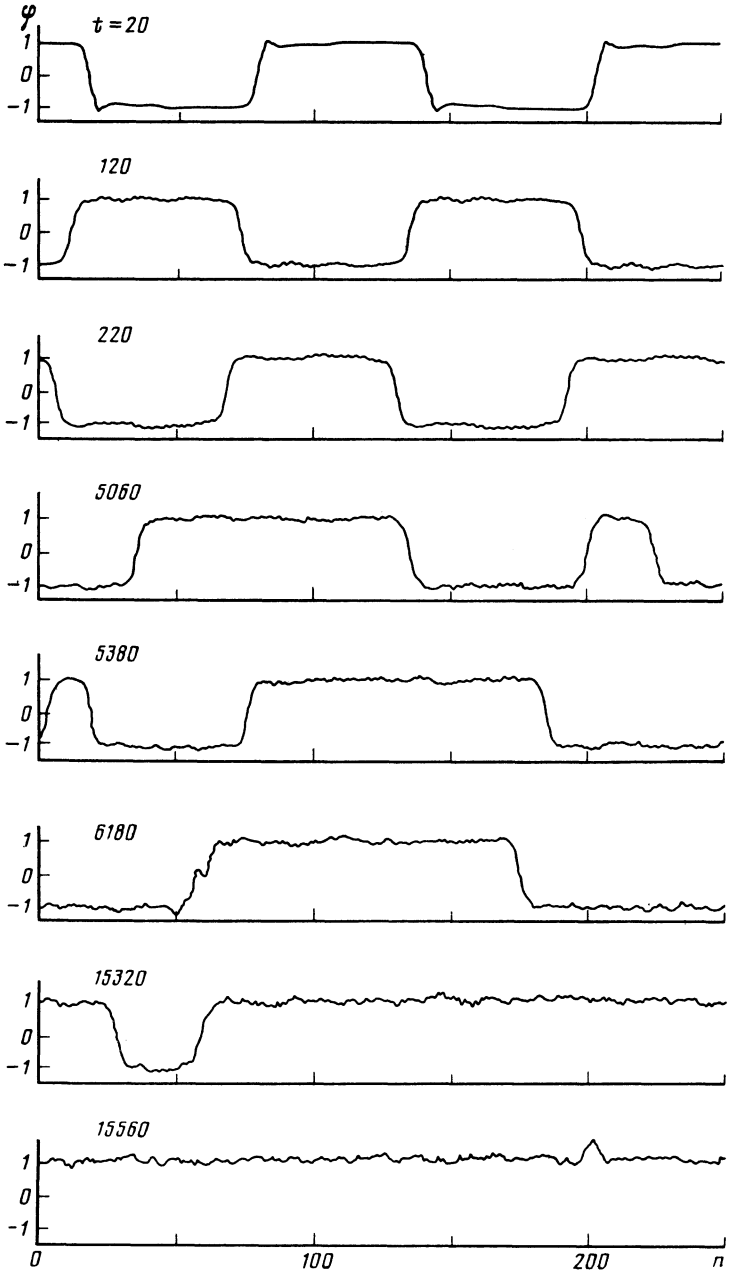

FIG. 5. Results of numerical integration of Eqs. (6) carried out on the assumption that $K = 0.05$ and $v = 0.005$.

their mutual approach and annihilation. After a finite time (in the present case, after $t \sim 15\,000$) this soliton structure is destroyed and only phonon-like excitations remain in the system. We integrated the system of equations (6) by the variable-order Adams method using variable steps. The precision of these calculations was controlled by retaining a constant energy integral $\mathscr{H} = \text{const}$ throughout a numerical experiment, and it amounted to 10^{-7}.

The results reported above on stable structures can be obtained also by a classical approach at zero absolute temperature. If we allow for finite temperatures and quantum effects, a numerical analysis of possible equilibrium configurations of the φ^4 model and of its stability become much more complicated. In the present study the influence of temperature and quantum fluctuations is discussed using the approximation of a self-consistent phonon field, which we employed earlier in a study of the FK model.[8,9] In this approximation the system of equations governing equilibrium positions of particles in a chain $\langle \partial \hat{\mathscr{H}} / \partial \hat{\varphi}_n \rangle = 0$, where the brackets denote averaging of an effective quadratic Hamiltonian, reduces to a system of equations $\partial \tilde{V} / \partial \varphi_n = 0$, where $\tilde{V}$ is the renormalized interaction potential:

$$\tilde{V} = \frac{1}{2} \sum_n (\varphi_{n+1} - \varphi_n)^2 + K \sum_n (\varphi_n^2 - 1 + 3 \langle \varphi_n^2 \rangle)^2 + 2K \sum_n \langle \varphi_n^2 \rangle (2 - 3 \langle \varphi_n^2 \rangle). \quad (8)$$

Equation (8) was derived using a pseudoharmonic approximation in which only the mean-square fluctuations were allowed for:

$$\tilde{V}(x) = \langle V(x+u) \rangle \approx \exp(\tfrac{1}{2} \langle u^2 \rangle \nabla^2) V(x).$$

In this approximation the spectrum of self-consistent excitations is found from the equations

$$\nu_s^2 e_n^{(s)} = \tilde{V}_{nn} e_n^{(s)} - e_{n+1}^{(s)} - e_{n-1}^{(s)}, \quad (9)$$

where

$$\tilde{V}_{nn'} = \frac{\partial^2 \tilde{V}}{\partial \varphi_n \partial \varphi_{n'}}, \quad \langle \varphi_n^2 \rangle = c \sum_{s=1}^{N} \frac{|e_n^{(s)}|^2}{\nu_s} \operatorname{cth} \frac{\nu_s}{\tau}, \quad (10)$$

$$c = \hbar / 2b^2 (m\gamma)^{1/2}, \quad \tau = 2T/\hbar\omega_0,$$

ν_s and $e_n^{(s)}$ are the eigenfrequencies and the eigenvectors of vibrations of atoms in the chain. The equations describing an equilibrium structure are then

$$I_{n+1} = I_n + 4K\varphi_n(\varphi_n^2 - 1 + 3\langle \varphi_n^2 \rangle), \quad \varphi_{n+1} = \varphi_n + I_{n+1}. \quad (11)$$

Equations (9)–(11) represent a closed system of equations determining the equilibrium positions of particles in a chain and the spectrum of their small vibrations.

It should be noted that inclusion of thermal and quantum fluctuations in this approximation renormalizes the one-particle potential, and this lowers the potential barrier separating the two wells. If this barrier is equal to K for $T = \hbar = 0$, and after allowance for fluctuations we find that $\tilde{K}_n = K(3\langle \varphi_n^2 \rangle - 1)^2$. Therefore, the influence of temperature and quantization reduces the parameter K. This means that the temperature and quantum effects lower the pinning force and the threshold for the annihilation of soliton–antisoliton pairs.

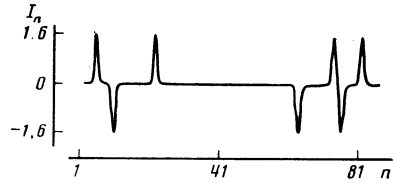

FIG. 6. Stochastic soliton structure obtained by solving Eqs. (9)–(11) on the assumption that $K = 6$, $c = 0.5$, and $\tau = 0$.

A numerical analysis of the solution of Eqs. (9)–(11) was made for a chain of 89 particles. At $T = 0$ and for the quantization parameter $c = 0.5$ we formed the random soliton structure shown in Fig. 6. This structure was obtained as a solution of Eqs. (9)–(11) by the method described in Refs. 8 and 9.

It should be noted that the solitons in Fig. 6 are much narrower and this is due to the fact that the parameter K is considerably greater ($K = 6$) and that soliton–antisoliton pairs are far from the conditions favoring annihilation. Heating a structure ($T \neq 0$) reduces the value of K; the first to be annihilated are soliton–antisoliton pairs separated by the shortest distances. The structure formed after annihilation of a soliton–antisoliton pair in the case when $\tau = 6$ is shown in Fig. 7. Therefore, our numerical analysis of stochastic soliton structures carried out using the discrete φ^4 model and allowing for thermal and quantum fluctuations predicts the annihilation of solitons and antisolitons which are of local nature. An increase in the temperature of a regular soliton structure causes annihilation of the pairs which is of global nature.

The results obtained on the local destruction of random structures are confirmed also by a numerical analysis carried out by the molecular dynamics method in the case of a chain consisting of 250 atoms. The initial conditions were in the form of a dynamically stable soliton structure shown in Fig. 8. All the atoms in the chain were assumed to have a certain initial velocity given by

$$\dot{\varphi}_n(0) = v_0 \sin(2\pi n \cdot 5/250), \quad n = 1 - N. \quad (12)$$

The Hamiltonian equations of motion (6) were solved subject to the free boundary conditions $\varphi_{N+1} = \varphi_N$, $\varphi_0 = \varphi_1$. In the case of sufficiently low initial velocities v_0 ($v_0 < 0.01$) the initial structure was found to be stable for all the times assumed in the numerical experiment. This was due to the fact that the kinetic energy imparted to the chain was insufficient to overcome the pinning barrier. An increase in v_0 revealed local melting processes (Fig. 8). Clearly, such a local melting process begins from soliton–antisoliton pairs with

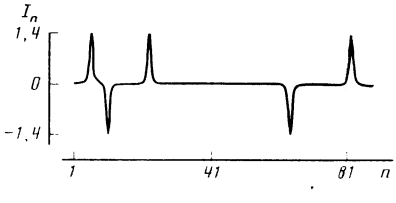

FIG. 7. Stochastic soliton structure at a finite temperature, calculated for $K = 6$, $c = 0.5$, and $\tau = 6$.

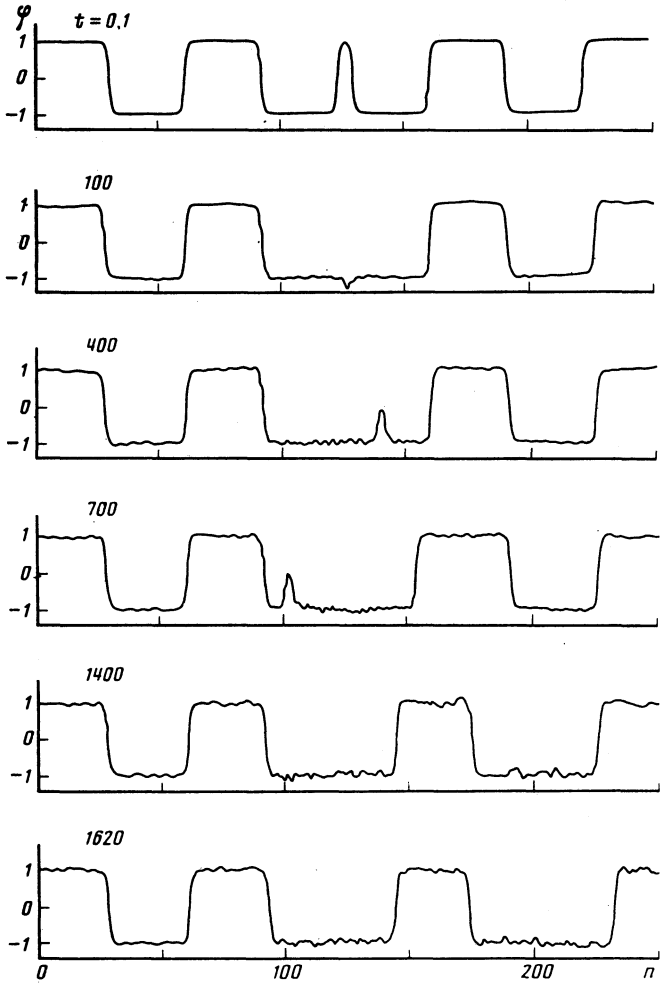

FIG. 8. Results of numerical integration of Eqs. (6) on the assumption that $K = 0.35$ and $v_0 = 0.11$ (free boundary conditions).

the shortest internal separation. After a long time there is a further annihilation of pairs.

The influence of thermal and quantum fluctuations on the structures predicted by the φ^4 model is different from that in the case of FK model. As shown in Refs. 8 and 9, fluctuations in the FK model result in local melting of a chain in soliton regions and not in the annihilation of soliton–antisoliton pairs. Numerical analysis of the spectrum of small vibrations of atoms in a soliton structure, carried out over a wide range of the parameter K (up to $K = K_{cr}$) revealed the existence of a finite gap and the absence of the phason mode. The latter implies that there cannot be any unpinned regular soliton configurations in the discrete φ^4 model, in contrast to the FK model. This conclusion is supported by the results of a numerical investigation of the equations of motion (6) carried out by the molecular dynamics method. In our numerical experiment a moving soliton structure was found to break up in a finite time as a result

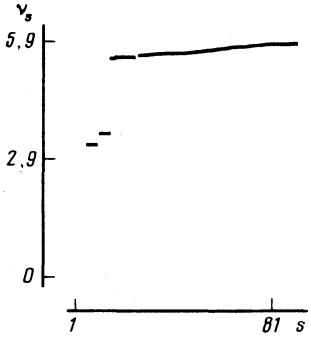

FIG. 9. Spectrum of small vibrations of a structure shown in Fig. 7.

of the soliton–antisoliton annihilation process.

Figure 9 gives an example of a spectrum of small vibrations of atoms in a structure shown in Fig. 7. The spectrum can be divided arbitrarily into three characteristic zones. The lower zone contains local symmetric vibrations of atoms in a soliton. The second zone also contains local vibrations, which are related to the soliton component and they represent a band of antisymmetric vibrations. The upper zone contains vibrations of atoms forming regular parts of the structure.

A numerical analysis of soliton structures in the discrete φ^4 model shows that there is a critical value of the parameter of the two-well potential K_{cr} (which depends on the soliton density) below which the soliton structure is dynamically unstable. For $K < K_{cr}$ the existing exponential attraction between solitons and antisolitons results in their mutual annihilation. The main manifestation of temperature and quantum effects in this model are an effective reduction in the parameter K and local annihilation of soliton–antisoliton pairs.

The authors are grateful to A. F. Sadreev for his interest and valuable comments.

[1]S. Aubry and P. Y. Le Daeron, Physica D (Utrecht) **8**, 381 (1983).
[2]P. Bak, Rep. Prog. Phys. **45**, 587 (1982).
[3]M. Peyrard and S. Aubry, J. Phys. C **16**, 1593 (1983).
[4]P. Y. Le Daeron and S. Aubry, J. Phys. C **16**, 4827 (1983).
[5]P. Bak and V. L. Pokrovsky, Phys. Rev. Lett. **47**, 958 (1981).
[6]A. S. Davydov, *Solitons in Molecular Systems*, Dordrecht, Boston (1985).
[7]V. V. Beloshapkin, G. M. Zaslavskiĭ, and A. G. Tret'yakov, Fiz. Nizk. Temp. **12**, 733 (1986) [Sov. J. Low Temp. Phys. **12**, 415 (1986)].
[8]V. V. Beloshapkin, G. P. Berman, A. M. Iomin, and A. G. Tret'yakov, Zh. Eksp. Teor. Fiz. **90**, 2077 (1986) [Sov. Phys. JETP **63**, 1217 (1986)].
[9]V. V. Beloshapkin, G. P. Berman, and A. G. Tret'yakov, Phys. Lett. A **124**, 90 (1987).
[10]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B **11**, 3535 (1975).
[11]A. F. Sadreev, Preprint No. 416F [in Russian], Institute of Physics, Siberian Division of the Academy of Sciences of the USSR, Krasnoyarsk (1987).

Translated by A. Tybulewicz