Soliton structure of lattice vibrations in a one-dimensional anharmonic chain

V. S. Zhukov
Ural Wood-Technology Institute

(Submitted 10 October 1983)
Pis'ma Zh. Eksp. Teor. Fiz. **38**, No. 11, 523–524 (10 December 1983)

Soliton and phonon excitations in a thermalized chain consisting of one hundred atoms interacting via an anharmonic Morse potential are separated with the help of the proposed method for two values of the total energy. The contribution of solitons to the energy of lattice excitations is determined.

PACS numbers: 63.10. + a

It is well known that a lattice of particles that interact according to a nonlinear law can have excited localized states in the form of solitary waves (solitons). On the other hand, in the classical approach, the thermal motion is viewed as a superposition of harmonic lattice vibrations (phonons). It is interesting to clarify how these two types of lattice excitations coexist in solids with interaction close to the real interaction. To solve this problem, it is proposed that they be separated with the help of a technique that consists of attaching a cold chain to a thermalized chain of atoms.[1] In the process of propagation of a thermal front, the soliton excitations overtake the front and become objects that are easily observable.

The lattice excitations were investigated by the method of molecular dynamics in a one-dimensional chain consisting of one hundred atoms which interact with each other via an anharmonic Morse potential. The numerical integration of the classical equations of motion of the particles was carried out using Beeman's finite-difference scheme.[2] The thermal motion was determined by assigning initial deviations and velocities to each atom with the help of a random number generator. Then, the particles

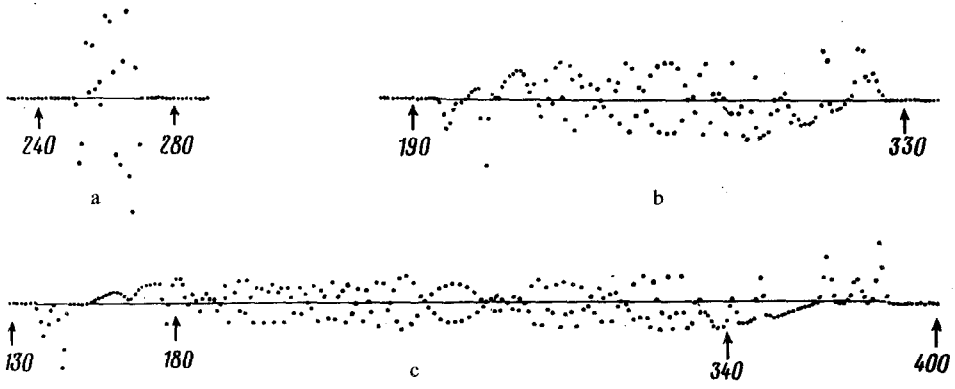

FIG. 1. Instantaneous velocities of atoms in the lattice. a — Initially, b — after 2000 times steps, and c — after 4000 time steps.

performed oscillations with periodic boundary conditions for several time steps in order to guarantee thermal equilibrium. The chain was then separated into five fragments with twenty atoms each and the analysis of soliton excitations was performed for each section separately. The fragment of the thermalized chain was included in the center of the cold chain consisting of 500 stationary atoms. Subsequently, the method of molecular dynamics was used to examine the propagation of thermal oscillations with time to the right and left along the lattice of 520 particles formed in this manner. The initial and subsequent conditions are shown in Fig. 1. Initially atoms with numbers from 251 to 270 oscillate. After 2000 time steps, the thermal motion encompasses sections of atoms with numbers from 200 to 320. Since the total energy of the system is conserved, as the number of oscillating particles increases, the average amplitude of the motion decreases. Solitary waves begin to appear in front of the thermal front. As a result, their velocity exceeds the velocity of the front. After 4000 steps, the soliton excitations become clearly visible. For the case shown in Fig. 1, the solitons which move to the left and which have negative velocities are located in the section of the chain with atoms numbered from 140 to 180, while the solitons which propagate to the right with positive velocities are located in the section numbered from 340 to 390. Elements of standing harmonic waves can be seen in the thermal motion of atoms at the center of the chain. Solitary waves moving in front of the thermal front have all the properties of solitons. Their amplitudes and shape remain unchanged with further propagation. The velocity depends on the amplitude. The solitary wave with a high amplitude overtakes the wave with a low amplitude without producing any mutual effect.

For a sufficiently large number of time steps, it may be expected that all solitons existing initially in the thermalized fragment have moved in front of the thermal front and the soliton and phonon lattice excitations have become spatially distributed. In this case, it is possible to calculate their energy separately, and to clarify the contribution of the soliton excitations to the total thermal energy of the thermalized lattice. Such an analysis and calculation were performed for two values of the total energy of

the chain per atom and scaled to the depth of the potential well of the interatomic interaction. An energy equal to 0.044 corresponds to the contribution of solitons equal to 0.26 and an energy of 0.254 corresponds to a contribution of soliton excitations equal to 0.39. Thus an increase in the energy of thermal vibrations, and their amplitudes, and therefore, the anharmonicity is accompanied by an increase in the contribution of solitons to the excitation energy of the lattice.

[1]J. Betteks and J. Powell, Solitony v deĭstvii (Solitons in Action), Ed. by K. Longren and E. M. Scott, Mir, Moscow, 1981.
[2]D. Beeman, J. Comput. Phys. **20**, 130 (1976).

Translated by M. Alferieff
Edited by S. J. Amoretty