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SOLITON ORGANIZATION OF THERMAL FIELD IN A CHAIN AT HIGH TEMPERATURE

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It has been shown that in a nonlinear chain the soliton organization of thermal field at high temperature, arising at the cost of absorption of background vibrations is possible. At some stage the intensive waves are formed and give energy distribution distinguished from the Maxwell-Boltzmann's one.

A phonon (the extended mode) delocalized in the coordinate space, but localized in the wave space is the fundamental quasi-particle in crystal reality. Since any of a number of phonons occupies the entire space of the crystal, each individual particle takes part in the motion of all the phonons. In the result of accidental phase combination of some phonon groups the multiphase and single-phase waves may arise with spatial localization of the order of the lattice spacing. In consequence of disperse features of the lattice they will be scattered prior to their wave properties are exhibited. With nonlinearity, phonon groups may form a long-lived bound states and in this situation the wave properties will be exhibited in full measure. The soliton-like excitations of two types, such as kinks and bell-form solitons [1–5], on the one hand, or breasers (gap solitons, intrinsic localized modes and so on) [5–9], on the other hand, observed in computer experiments for different nonlinear lattices, directly confirm this fact. The former may exist below the linear phonon band, the latter ones above the upper harmonic phonon band edge, that is inside the gap [6] or inside the self-induced gap [7].

Nonlinear waves of different nature manifest a series of common properties including suppression and absorption of small waves by larger ones. In Ref. [9] such phenomenon was observed for small and large exact breasers. In Ref. [10] the chaotic breasers were observed in the numerical experiment for the FPU-chains, which manifest the effect of energy concentration by separate excitations. As the initial condition the π-mode was taken. It is shown that the π-mode decays into local excitations with chaotic behavior. In the initial stage the concentration of energy by separate breasers grows. Later on, these excitations vanish and the system approaches the equipartition state. The authors state that the pumping of energy from the high-frequency π-mode to the low-frequency region of phonon spectrum takes place in this way.

After relaxation the chaotic breasers die out because of «starvation». This brings up the question: is such behavior of a system, when the chaotic breasers do not die out and rest after the relaxation, possible? To achieve such regime it is necessary, that the mean energy per one particle, that is, temperature, be high enough. The localization modes are regarded also for FPU-chains in numerical experiment of Ref. [11].

The aim of this paper is to investigate similar effects for kink solitons at high temperature and their influence on thermal field by means of computer simulation. To minimize the non-equilibrium pumping effect here the «white noise» distribution is used as the initial state. The «white noise» is energy distribution closest to thermodynamic equilibrium state. One may expect that the relaxation passes fast enough.

It should be noted that a FPU-chain is a very idealistic model for atomic systems and it deviates from realistic ones to a greater extent with the vibration amplitude increase. In our case such a situation presents the main interest for the investigation. It follows that one of the realistic potentials containing non-linearity of all orders must be used for such system at high temperature.

All simulation was performed for a chain built up of 200 particles interacting via the most popular 6–12 Lennard-Jones' potential, that is

$$U_{ij} = u_{\min}\left[\left(\frac{r_0}{r_{ij}}\right)^{12} - 2\left(\frac{r_0}{r_{ij}^6}\right)^6\right], \qquad (1)$$

where $r_{ij} = \sqrt{(X_i - X_j)^2 + (Y_i - Y_j)^2}$ – is the distance between particles with numbers i and j, and Cartesian coordinates X_i, Y_i, X_j, Y_j, r_0 – is the equilibrium distance for two-particle systems, $u_{\min}$ – is the binding energy. For the sake of simplicity the reduced units of length and time as $\tilde{r}_{ij} = r_{ij}/r_0$ and $\tilde{t} = t/T$, respectively, are defined. Here $T = 2\pi m/U''_{ij}(0)$ is the period of small vibrations, m is the particle mass which equals unity thereafter. The binding energy in the reduced units turned out to be equal to $2(\pi/6)^2$. A smaller than T conventional unit of time must be introduced for the description of wave phase. We take it to be equal to $t_{\text{con}} = 0.005$ (time step in the computer experiment). For calculation the sixth-order Yoshida's symplectic algorithm is used [12]. The law of conservation of energy is fulfilled to a relative accuracy of 10^{-6}.

The equilibrium state is determined by coordinates $X_i^{(0)}$, $Y_i^{(0)}$:

$$X_i^{(0)} = r_0 i, \qquad Y_i^{(0)} = \text{const}. \qquad (2)$$

The initial distribution of particle velocities is chosen in the form of white noise with amplitude 4.078 for X-polarization only. The initial disturbances along Y-direction was not preset, however, for additional control over computer errors the movement in this direction was permitted. The average additional energy per one particle contributed by white noise turned out to be equal to 2.6895 of reduced units. This value is 4.9 times as much as the binding energy. Such correlation of energies corresponds to high enough temperature of the chain which is much higher than the melting point.

The evolution of white noise in time for a chain built up of 200 particles is presented by four graphic fragments. Every fragment is composed of 46 constitutive spatial profiles reflecting the square of particle velocity or kinetic energy versus its number in the chain. In its turn, every constitutive profile is formed, by graphic superposition, of ten elementary profiles taken during ten time steps. Such display permits one to improve the tracing of waves for a long time.

Really, as would be expected, the early stage of evolution (the lower fragment in Fig. 1) is very close to homogeneous distribution. Nevertheless, at this stage the local excitations with size of the order of lattice spacing are traced already. These local objects conserve their shape both at free spreading, and after interactions in between for a long time. Their velocities determined by slope of traces vary from 10 to 16 of reduced units and they turn out to be proportional to wave amplitude. A consequence of the above is the fact that we deal with the soliton-like waves.

From general considerations it is quite evident that they are the soliton-like objects of kink kind. Really, if spreading of excitation is presented as consecutive frontal collisions of particles, then in the result of a separate collision a moving particle stops and the resting particle starts to move with the same velocity. In the next collision this moving particle stops too in a new position, and so on. As a result, we have the switching wave of the kink type. Evidently, in our case we have a multitude of such waves, interacting, in addition, with each other.

By virtue of white noise proximity to the equilibrium state it may seem that the relaxation will pass sufficiently fast. However, the next, second fragment on the bottom of Fig. 1 testifies that the system approaches equipartition state, but deviated towards even greater inhomogeneity of the spatial distribution of particle velocities. In the chain the high-amplitude waves arise, concentrating a significant part of system energy. As the law of energy conservation is fulfilled with high precision, this can be traced at the cost of energy re-distribution among the excitations, namely, high excitations have captured the energy of the low ones. This phenomenon is analogous to the decay of the π-mode into the chaotic breasers [10]. The surprising thing is that almost identical effect ac-

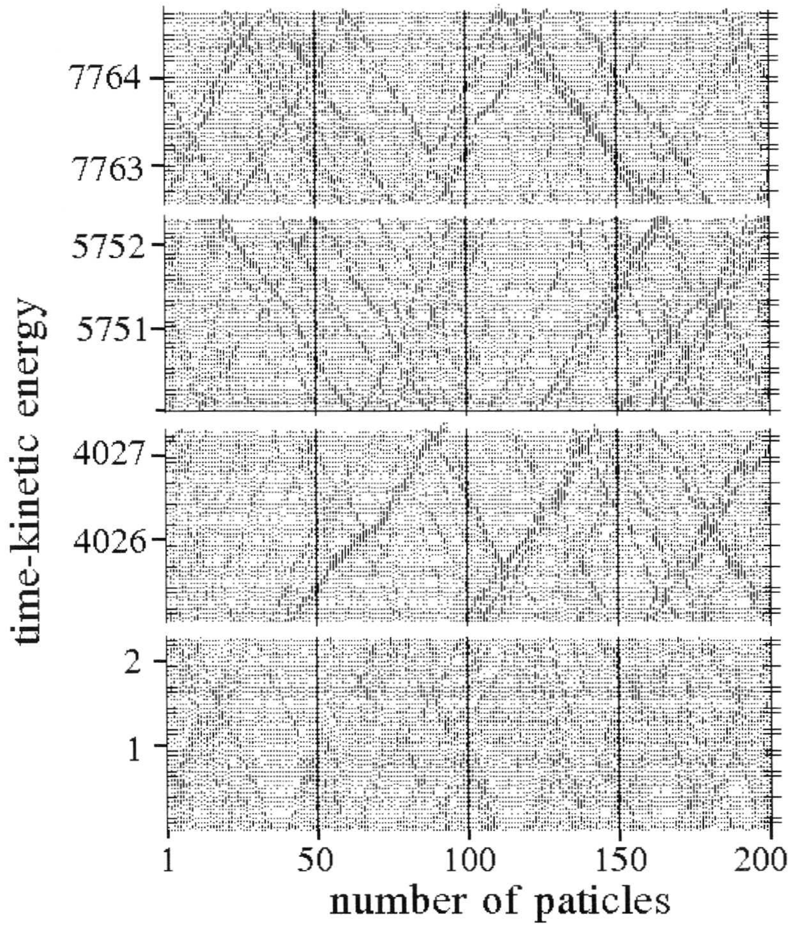

Fig. 1. Evolution of white noise: reading of time along vertical axis goes in reducing units

companies the breakdown of white noise. Next two fragments (Fig. 1) show that the level of inhomogeneity of the velocity field varies in time, however, in any event, it is considerably above than that at the starting stage (the uppermost fragment). This inhomogeneity doesn't vanish at high time of system evolution and, it is obvious that it doesn't vanish at all. Thus, while in the Ref. [10] chaotic breasers were an interface at system relaxation and they vanished after the achievement of thermal equilibrium, in our case the soliton-like excitations are the main objects of the equilibrium thermal field. This permits one to conclude that solition organization of thermal field takes place in such situation.

To support this conclusion let us correlate «real» distribution of particle energy with theoretical Maxwell-Boltzmann's one. In Fig. 2 the curves with circles correspond to «real» data of the numerical experiments, solid ones correspond to theoretical distribution: Descending curves describe a distribution of particles by energy n_i, determined as number of particles with energy $(i - 1)\Delta\varepsilon \le \varepsilon < i\Delta\varepsilon$, where i – is the number of interval. The curves with one or many peaks are the energy spectra E_i, determined as total energy of particles in the same interval. Theoretical equilibrium distribution of this quantities are of the form:

$$n_i = n_0 \exp(-\varepsilon_i/\theta), \quad E_i = \varepsilon_i n_i \tag{3}$$

with the fulfillment of laws of conservation for particles and energy:

$$N = \sum_{i=1}^{\infty} n_i, \quad E = \sum_{i=1}^{\infty} \varepsilon_i n_i, \tag{4}$$

where n_0 – is the number of particles with minimum energy, θ – is temperature in the energy representation of reduced units.

From the last relations the expressions for n_0 and θ follow:

$$\theta = E/N, \quad n_0 = N^2/E. \tag{5}$$

All graphs built with numerical experiments are obtained by means of averaging over 460 time steps and they correspond to fragments in Fig 1. Energy interval $\Delta\varepsilon$ used at building of graphics was taken to be equal to 1.6 of reduced units.

One can see from the first graph that the white noise deviates from Maxwell-Boltzmann's distribution to a greater extent than any in Fig. 2. On the energy spectra for real data the peak has higher value than for theoretical ones at the cost of a fraction of low-energy excitations. The particles with high energy are

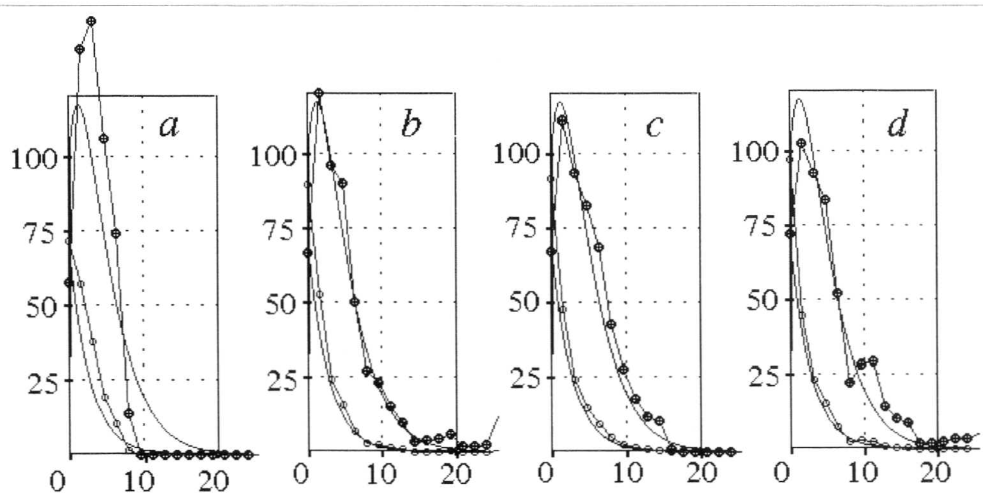

Fig. 2. Real and theoretical distributions of particles and energy spectra versus the energy

absent in the system at all. With the evolution of white noise the energy is pumped from the second graf in Fig. 2 that the first peak has decreased below theoretical value while additional peaks have arisen in the high-energy region. In this region the energy curve lies markedly higher than the theoretical one. With later evolution (the third graph in Fig. 2.) a peculiar kind of returning is observed, namely, real distribution achieves the theoretical one. Additional have vanished. It should be noted that such equilibrium deffers in the nature of its organization from a phonon variant [10]. Really, in our case (see the third fragment in Fig. 1.) local excitations continue to exist during all the time. This is the principal new finding.

One may expect that the system having achieved, finally, the thermal equilibrium, well rest in this state for a long time. However, the further evolution of the system (see the fourth graph in Fig. 2) shows that with time the system returns to the state with additional peaks again. At the same time the returning can't be considered as simple fluctuation, since it develops directly and sequentially during a long time of about 300–500 reduced units of time. Later on, both of these states alternate in time.

The departure of equilibrium distribution from the Maxwell-Boltzmann's one is marked in Ref. [3] for chock waves in one-dimensional chains. If θ_0 is the initial temperature and θ is the final temperature ahead and behind of the chock front, respectively, then the equilibrium distribution of the particle velocities is determined by the following expression [3]:

$$n_i = \frac{1}{2}(2\kappa\theta)^{-1/2}\left[\exp\left(-\frac{\left(v_i - \vartheta^{1/2}\right)^2}{2\theta_0}\right) + \exp\left(-\frac{\left(v_i + \vartheta^{1/2}\right)^2}{2\theta_0}\right)\right], \quad (6)$$

where $\vartheta = \theta - \theta_0$, v_i – is velocity of a particle, or with regard of potential energy contribution

$$n_i = \bar{n}_0 \exp(-\varepsilon_i/\theta_0)\mathrm{ch}(2\varepsilon_i\vartheta)^{1/2}, \quad (7)$$

where $\bar{n}_0 = n_0\exp(-\vartheta/2\theta_0)$, $n_0 = (2\pi\theta_0)^{-1/2}$ – is the same n_0 as in expression (3).

One may see that at $\vartheta > 0$ $\bar{n}_0 < n_0$ is true, that is, the number of particles with minimum energy is less then that for the Maxwell-Boltzmann's distribution. At the same time, owing to factor $\mathrm{ch}(2\varepsilon_i\vartheta)^{1/2}$ a share of the high-energy particles grows. The same is true for energy spectrum.

From third graph in Fig. 2 one can see, that the «real» distribution being qualitatively described by expression (7) is formed in the system. However, no peaks in the spectra in Fig. 2,*b*,*d* are described by this expression. The emergence of the ones is a quantitatively new peculiarity of a nonlinear system at high temperature. Its emergence is obviously connected with the long-living local high-energy excitations.

Thus, the described computer experiment has shown that the fundamental soliton organization of thermal wave field is possible at high temperature. Such phenomenon has led to spontaneous production of intensive nonlinear waves, which can be considered as a peculiar kind of self-organization of the thermal field. Investigation of this phenomenon is important to gain a better understanding of the break of a solid.

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