LIMITING PHASE TRAJECTORIES AND DYNAMICAL TRANSITIONS IN THE NONLINEAR PERIODIC SYSTEMS

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ABSTRACT

The efficient energy exchange in the nonlinear periodic Frenkel-Kontorova and Klein-Gordon lattices has been studied in the framework of the concept of Limiting Phase Trajectories proposed earlier. Two dynamical transitions occur while the nonlinearity of interaction grows. The first of them is connected with the lowest frequency normal mode bifurcation that leads to its instability and appearance of two new nonlinear normal modes. In the principal asymptotic approximation corresponding stationary points at the phase plane are circled by separatrix. However, a complete energy exchange between different parts of the system remains yet possible. The second dynamical transition corresponds with coalescence of separatrix and LPT that leads to prohibition of the energy transfer from one part of the system to another one. As the result, the energy input in some part of the system is confined in it. The results of analytical study are in accordance with computer simulation data

INTRODUCTION

Nonlinear dynamics of many-particle systems is a one of the key directions of the contemporary science [1]. The researches in this area give numerous surprising results. The one of the most wonderful and widely studied phenomena is the existence of localized excitations in the spatially uniform systems in which a uniform energy distribution should be expected *a priori*. Such self-organized localized states which are not induced by any intrinsic inhomogeneity or any external impact play an essential role in many dynamical processes relating to solid state physics and chemistry. Particularly, the most of qualitative transitions associated with chemical processes or structural transformations in the large molecules and crystals happen via the energy localization.

On the other side in the linear limit the systems under consideration demonstrate the dynamical behavior which is well described with using the Linear Normal Modes (LNMs). Their specific property is the absence of any intermodal interactions. In such limit the system turns out to be completely integrable that allows the exact description of its evolution. The concept of normal modes can be extended to nonlinear systems, and then they can be denoted as Nonlinear Normal Modes (NNMs) [2-7]. The exact determination of NNMs is an enough complicate problem; therefore their approximate representation may be useful, in particular in connection with the problem of energy localization in the reciprocal space of the system [8, 9].

However, one can see that both LNMs and NNMs are non-appropriate for the description of the process in which the intensive energy exchange or transfer along the chain occurs because the normal modes preserve the energy put into them. The processes of the energy transfer require the formation of wave packet which contains several NNMs and the number of NNMs in the packet increases if the localization becomes more distinct. To avoid the dispersive packet spreading the intermodal interaction associated with the nonlinear part of the potential energy is necessary. However the origin of the energy localization in oscillatory chains has not been still clarified.

In this paper we show that the analysis of a minimal wave packet containing the zone-boundary mode and nearest one in the discrete model of the sin-Gordon or Klein-Gordon chains leads

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to correct description of the energy localization in terms of "effective oscillators". Then the "beating" phenomenon observed in the small-amplitude limit is associated with the energy transfer from one half of the chain to another one. This phenomenon is described as the motion along the phase trajectory which bounds the attraction area of the zone-boundary normal mode (we call this trajectory as the Limiting Phase Trajectory – LPT; it was earlier introduced for weakly coupled oscillators [10-11] and for Fermi-Pasta-Ulam chain [12-14]). When the excitation level increases the topology of the phase space of the system is changed. We show that the first dynamical transition occurs when the zone-boundary mode turns out to be unstable, but the full energy exchange is possible yet. This transition is accompanied by the creation of two new stationary points (nonlinear normal modes which have not any analog in the linear spectrum of the system) which correspond to the partially localized states. The second dynamical transition changes the phase space of the system drastically: the LPT becomes discontinued and no trajectories associated with complete energy exchange between two parts of the chain occur. After this transformation of the phase space of the system the energy input in some part of the system is confined in it.

THE MODEL

Let us consider the nonlinear chain containing the N particles with the periodic boundary conditions. The respective Hamiltonian can be written as follows:

$$H = \sum_{j=1}^{N} \frac{p_j^2}{2} + \frac{c^2}{2}(q_{j+1} - q_j)^2 + V(q_j) \tag{1}$$

where the potential function

$$V(q) = \omega_0^2 (1 - \cos(\frac{2\pi}{d} q)) \tag{2}$$

corresponds to the Frenkel-Kontorova model and

$$V(q) = \frac{\omega_0^2}{2} q^2 + \frac{\beta}{4} q^4 \tag{3}$$

corresponds to the Klein-Gordon chain.

The linearized spectrum of eigenvalues is described as

$$\omega_k^2 = \omega_0^2 + 4c^2 \sin^2 \frac{\pi k}{N} \tag{4}$$

Introducing the normal modes

$$q_j = \sum_{k=0}^{N-1} \sigma_{j,k} \xi_k$$

with

$$\sigma_{j,k} = \frac{1}{\sqrt{N}} (\sin \frac{2\pi k j}{N} + \cos \frac{2\pi k j}{N}),$$

one can see that the lowest-frequency normal mode ($\omega = \omega_0$) corresponds to the uniform energy distribution the ξ_k being the amplitude of the k-th NM. As it was mentioned above we would like to analyse the minimal wave packet containing the low-frequency zone-boundary mode (k=0) and the mode belonging to nearest integral manifold (k=1). It is easy to show that such a combination leads to the energy distribution profile in which the main part of the energy is concentrated in the one half of the chain. Taking to account the mentioned NNMs only, we can write the potential energy up to four order as follows:

$$U[\xi_0, \xi_1] = \frac{1}{2}(\omega_0^2 \xi_0^2 + \omega_1^2 \xi_1^2) + \frac{\beta}{2N}(\frac{1}{2}\xi_0^4 + 3\xi_0^2 \xi_1^2 + \frac{3}{4}\xi_1^4) \tag{5}$$

(The Frenkel-Kontorova model is associated with the negative (soft) nonlinearity β<0 and the Klein-Gordon chain –with positive (hard) one β>0.)

One should note that the frequency difference

$$\omega_1 - \omega_0 = \sqrt{\omega_0^2 + 2c^2 \sin^2 \frac{\pi}{N}} - \omega_0 \approx \frac{2c^2 \pi^2}{\omega_0 N^2} << 1 \tag{6}$$

at N~10.

Now we can introduce the complex variables corresponding to normal modes [15]:

$$\Psi_k = \frac{1}{\sqrt{2}}(\frac{d\xi_k}{dt} + i\omega_k\xi_k), \quad \Psi_k^* = \frac{1}{\sqrt{2}}(\frac{d\xi_k}{dt} - i\omega_k\xi_k)$$

and use the multiple scale expansion:

$$\Psi_k = \Phi_k e^{i\omega_k t} = \sqrt{\varepsilon}(\chi_k + \varepsilon\chi_{k,1} + \varepsilon^2\chi_{k,2} + ...)e^{i\omega_k t}$$

$$\tau_0 = t, \tau_1 = \varepsilon\tau_0, \tau_2 = \varepsilon^2\tau_0,...$$

(7)

After some algebra we get the following equations describing the main order amplitudes dynamics by small parameter [13-14]:

$$i\frac{\partial\chi_0}{\partial\tau_2} + \frac{3\beta}{4\omega_0^3}[|\chi_0|^2\chi_0 + 2|\chi_1|^2\chi_0 + \chi_0^*\chi_1^2] = 0$$

$$i\frac{\partial\chi_1}{\partial\tau_2} + \nu\chi_1 + \frac{3\beta}{8\omega_0^3}[3|\chi_1|^2\chi_1 + 4|\chi_0|^2\chi_1 + 2\chi_1^*\chi_0^2] = 0$$

(8)

Eqs (8) correspond to the Hamiltonian

$$H_\chi = \nu|\chi_1|^2 + \frac{3}{16}\frac{\beta}{\omega_0^3}[2|\chi_0|^4 + 3|\chi_1|^4 + 8|\chi_0|^2|\chi_1|^2 + 2(\chi_0^2\chi_1^{*2} + \chi_0^{*2}\chi_1^2)]$$

(9)

and allow the additional integral of motion named "occupation number":

$$X = |\chi_0|^2 + |\chi_1|^2$$

(10)

As it was mentioned above the χ-variables are not convenient ones for the description of energy transfer. Therefore one should introduce the new variables which correspond to the "effective oscillators" as each of new variables describes the energy distribution concentrated at one half of the chain [14]:

$$\varphi_0 = \frac{1}{\sqrt{2}}(\chi_0 + \chi_1), \quad \varphi_1 = \frac{1}{\sqrt{2}}(\chi_0 - \chi_1)$$

$$|\varphi_0|^2 + |\varphi_1|^2 = X$$

(11)

Because the value X is the integral of motion it is convenient to rewrite the φ-functions as follows:

$$\varphi_0 = \sqrt{X}\cos\theta e^{i\delta_0}, \quad \varphi_1 = \sqrt{X}\sin\theta e^{i\delta_1}$$

(12)

where the angular variables allow us to study the phase plane of the system [16]. Then the equations of motion can be written in the form:

$$\sin 2\theta\frac{\partial\Delta}{\partial\tau_2} - \frac{\cos 2\theta}{16\omega_0^3}[(3\beta X + 16\nu\omega_0^3)\cos\Delta - 3\beta X\cos^2\Delta\sin 2\theta + 27\beta X\sin 2\theta] = 0$$

$$\sin 2\theta[\frac{\partial\theta}{\partial\tau_2} - \frac{1}{32\omega_0^3}(3\beta X + 16\nu\omega_0^3 - 3\beta X\cos\Delta\sin 2\theta)\sin\Delta] = 0$$

$$\Delta = \delta_1 - \delta_0$$

(13)

There are two stationary points at the small level of occupation number X (fig.1). The first of them (Δ=0, θ=π/4) corresponds to the zone-boundary mode (k=0) and the second one (Δ=π, θ=π/4) describes the nearest mode (k=1). The LPT is the trajectory which consists of two branches surrounding the attraction areas of both modes. It is easy to show that the φ$_0$ and φ$_1$ correspond to the parts of LPT which pass through the states θ=π/2 and θ=0, respectively. So the motion along the LPT is accompanied with the transfer energy from one half of the chain to another. This process looks like

the beating in the system of two weakly coupled oscillators. One should note that this phenomenon has to manifest itself beginning from the linear limit.
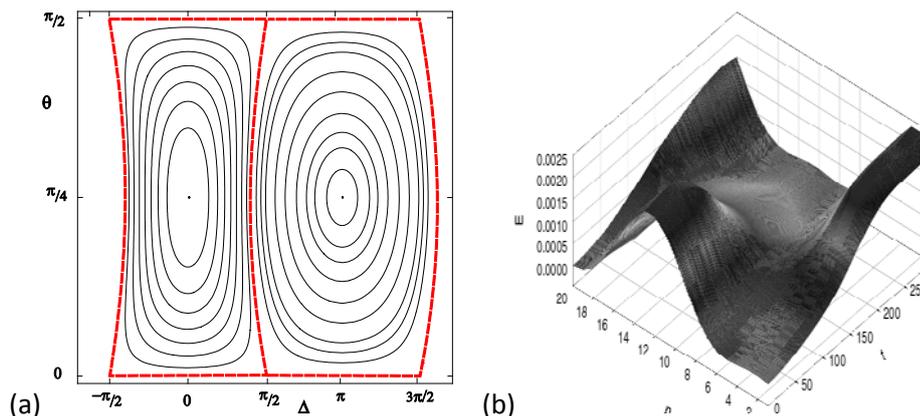

Fig.1 The phase plain portrait (a) and the 3D plot of the energy (b) of the FK-chain with 20 particles with two excited modes in the terms of angular variables.

While the excitation level grows the topology of the phase plane is changed. Two new stationary points

$$(a) \quad \begin{cases} \sin 2\theta = -\dfrac{3\beta X + 16\nu\omega_0^3}{24\beta X} & (FK-chain) \\ \cos\Delta = 1 \end{cases}$$

$$(b) \quad \begin{cases} \sin 2\theta = \dfrac{3\beta X + 16\nu\omega_0^3}{24\beta X} & (KG-chain) \\ \cos\Delta = -1 \end{cases}$$

(15)

arise in the phase plane because the zone-boundary mode turns out to be unstable at the excitation level corresponding to critical values

$$(a) \quad X_{cr} = -\frac{64\pi^2 c^2 \omega_0^2}{27\beta} \quad (\beta < 0)$$

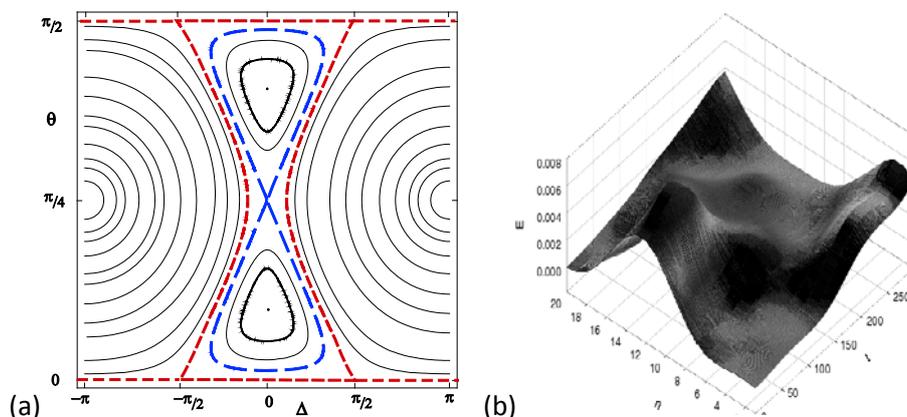$$(b) \quad X_{cr} = \frac{64\pi^2 c^2 \omega_0^2}{15\beta} \quad (\beta > 0)$$

(16)

Fig.2 The phase plane portrait (a) and the 3D plot of the energy (b) of the FK-chain with 20 particles above the first excitation threshold X_{cr}.

These new stationary points correspond to new nonlinear elementary excitations which describe the partially localized states when only some part of the energy of the system is concentrated in the one half of the chain the rest of the energy being distributed uniformly along the chain. The

separatrix that surrounds the attraction area of the new stationary point separates the phase plane into the domains where the complete energy exchange is forbidden (inside the separatrix) and where it is possible yet (out of the separatrix). The further growth of the excitation is accompanied with decreasing of domain corresponding to complete energy exchange and this domain becomes degenerate when the energies of LPT and unstable stationary point ($\theta=\pi/4$) turn out to be equal:

$$E(\theta = \pi/4, \Delta = 0) = E(\theta = 0, \Delta = 0)$$

where the energy is defined by the Hamiltonian in the angular variables:

$$H = \frac{X}{256\omega_0^3}[159\beta X + 128\nu\omega_0^3 + 45\beta X \cos 4\theta - 8(3\beta X + 16\nu\omega_0^3)\cos\Delta\sin 2\theta + 6\beta X \cos 2\Delta\sin^2 2\theta]$$

The respective values of occupation number X are equal to:

$$(a) \quad X_t = -\frac{64\pi^2 c^2\omega_0^2}{27\beta} \quad (FK-chain)$$

$$(b) \quad X_t = \frac{64\pi^2 c^2\omega_0^2}{15\beta} \quad (KG-chain)$$

$$(17)$$

The Fig.3.a shows that the topology of phase plane is change drastically: no trajectory started near the amplitude value $\theta=0$ ($\theta=\pi/2$) can not approach to the value $\theta=\pi/4$ that means the absence of complete energy exchange between two parts of the chain. Moreover, the maximal localization turns out to be possible when the main part of the energy is confined in the one part of the chain. This phenomenon is clearly seen in the fig. 3b. The periodic variation of the energy distribution (so called "breathing" mode) is correlated with the traveling along the phase trajectory surrounding the stationary points (17.a) or (17.b).
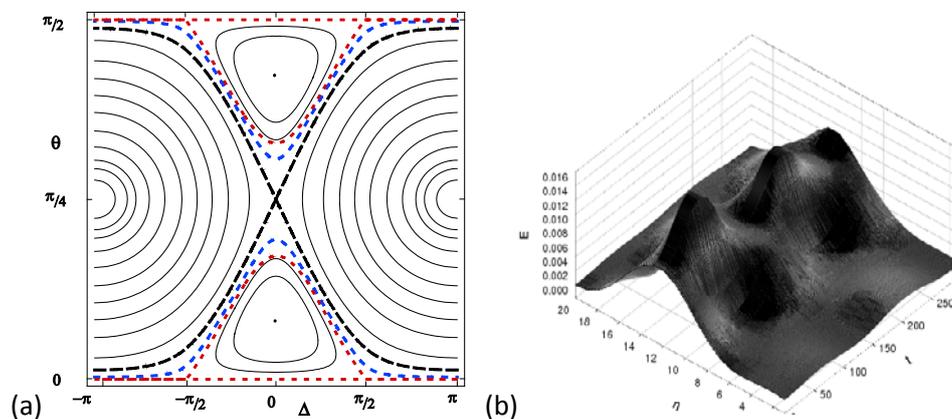

Fig.3 The phase plane portrait (a) and the 3D plot (b) of energy for the FK-chain with 20 particles above the threshold of localization Xt.

One should point the essential difference between FK and KG chains that becomes apparent at the threshold of the localization. The localization occurs in the FK chain if the excitation level exceeds the value X_t, while the dynamics of KG-chain demonstrates the partial localization only. This difference results from the fact that the unstable mode in the FK-chain is the zone-boundary one while the nearest to zone-boundary mode turns out to be unstable in the KG-chain. The figures 4(a-c) illustrate the results described above.

It is clearly seen that high energy area jumps from n=20 to n=5 (beating phenomenon) if the occupation number X is smaller than the localization threshold X_t and it is confined at n=20 if X has overcame the threshold of localization. The lighter regions dividing the nearest dark ones are

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associated with passing of representation point near the $\theta=\pi/4$ in the reduced phase plane (see figs 1-3). Thus one can explain the origin of "breathing" mode of the localized vibrations (breathers).
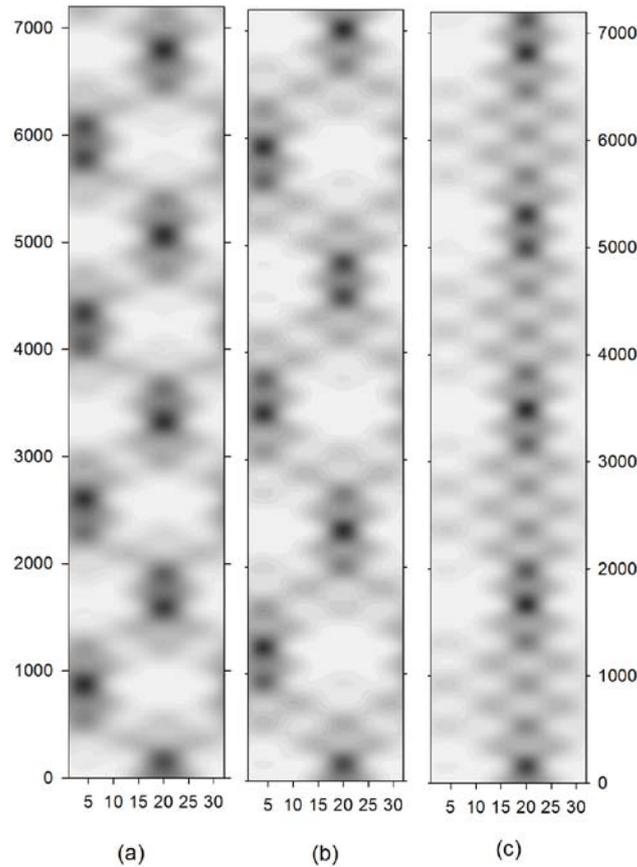

Fig.4. Energy contour map for the FK-chain with 32 particles at various values of occupation number X: (a) $X<X_{cr}$, (b) $X_{cr}<X<X_t$, (c) $X_t<X$. The horizontal and vertical axes correspond to the particle's number and the time measured in the oscillation period of low-frequency zone-boundary mode, respectively. Darker regions correspond to oscillators with more energy, lighter regions to oscillators with less energy.

CONCLUSION

The analysis made above has shown that the origin of the energy localization in the nonlinear chains is the resonant interaction of the NNMs corresponding to the edge of the linear spectrum. At that, the loss of stability of the zone-boundary mode is the necessary but not sufficient condition for complete energy localization. This instability leads to arising two new stationary points corresponding to the states with only partial energy localization while the complete localization turns out to be possible after the second dynamical transition (when the domain of the phase trajectories associated with the full energy exchange becomes degenerate and the LPT is discontinued. The last results in forbidding the complete energy exchange between different parts of the chain (the energy put in the some part of the chain is confined in it). One should note that this simplified description taking into account two boundary modes only reflects the principal peculiarities of the process. As the computer simulation data show, the presence of other modes leads to some narrowing of the profile of the energy distribution, but does not change the main features of the process. It can be shown that an similar scenario of energy localization is valid for the high-frequency edge of the spectrum, but at that the KG chain trends to the energy localization while the FK chain does not do it. One should note that the critical density of the energy is inversely to the square of the particle number and it converges to zero when the number of particles go to infinity.

In conclusion we would like to make one more remark concerning the LPT and the notice of "effective oscillator". As it was mentioned in the Introduction, the description of energy localization in the terms of the NNMs is not adequate one because they turn out to interact strongly near the localization threshold. Therefore, the introduction of the new objects which can be defined well and the interaction between which is weak is the adequate procedure to describe the process under consideration. In the case considered the "effective oscillators" are two halves of the chain. Therefore,

the LPT is the phase trajectory which describes the energy exchange between two "effective oscillators".

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