ROLE OF ENERGY EXCHANGE IN THE DETERMINISTIC ESCAPE OF A COUPLED NONLINEAR OSCILLATOR CHAIN*

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We consider the deterministic escape of a chain of harmonically coupled units from a metastable state over a cubic potential barrier. The underlying dynamics is conservative and noise-free. The supply of a sufficient total energy transforms the chain into the nonlinear regime from which an initially, nearly uniform lattice configuration becomes unstable, yielding a redistribution of energy. In an early stage of the dynamics, we estimate the degree of energy exchange enabling the coupled system to form strongly localized modes which eventually grow into a critical nucleus. Upon passing this transition state, the nonlinear chain performs a collective, deterministic escape. We analyze the associated nonlinear dynamics in phase space and relate the escape to diffusion in a separatrix layer.

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1. Introduction

Ever since the benchmark work by Kramers [1] (for a comprehensive review see in Ref. [2]) there is a continued and growing interest in the dynamics of escape processes of single particles and of coupled degrees of freedom out of metastable states. Escape is realized by the passage of the considered objects over an energetic barrier which separates the local potential minimum from a neighboring attracting domain.

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There is implied that the system is in contact with an external heat bath serving as a permanent source of energy, causing dissipation and local energy fluctuations which successfully enable the escapes. Many generalizations of Kramers escape theory in over- and underdamped versions have been widely exploited [2]. Nowadays, this approach is commonly utilized in biophysical contexts and for a great many applications occurring in physics and chemistry [3–14].

The noise-free microcanonical situation has been studied less intensely. Then, the system cannot feed on an external energy source but rather a fixed amount of energy has to suffice to perform a barrier crossing.

Such deterministic escape process of an one-dimensional coupled oscillator chain has been presented as robust — and purely self-organized — barrier crossing mechanism [15–17]. The absolutely necessary ingredients in the physics of these deterministic barrier crossings are nonlinear potentials wherein the chain moves and the discreteness of the chain units. Both avert the chain to relax to states with equipartition of energy among its constituents. In contrast they allow localization of a sufficient amount of energy on a few oscillators forming a critical state.

An escape is related with a crossing of a saddle point in the configuration space, corresponding to bottlenecks [2]. We shall assign a critical energy to this transition state E_{crit} which has to be concentrated at the critical mode. It was shown [15–17] that the latter can be reached in the microcanonical situation spontaneously. In particular, it was found that intrinsic nonlinear effects on a long discrete chain of N units induce a transition over an energetic barrier by enhancing one, or several localized breather states [18–26]. With this mechanism an initially almost uniformly distributed energy can become dynamically concentrated by internal redistribution without the need of an assistance of energy supply of a thermal bath.

The present work aims to gain further insight into the self-organized deterministic escape processes presented in [15–17]. In the next section we introduce the model of the coupled oscillator chain. We focus our interest on low-energy modes corresponding to nearly equilibrium states of the lattice chain. The properties of localization induced by the dynamical formation of breather arrays are explored in Sec. 3. Finally in Sec. 4 the escape process is characterized as diffusion in an associated stochastic separatrix layer in phase space.

2. Coupled oscillator chain model

We study a one-dimensional lattice of coupled nonlinear oscillators. The coordinate q of each individual oscillator evolves in a cubic single well potential of the form

$$U(q) = \frac{\omega_0^2}{2} q^2 - \frac{a}{3} q^3 \,. \tag{1}$$

This potential possesses a metastable equilibrium at $q_{\min} = 0$ corresponding to the rest energy $E_{\min} = 0$ and the maximum is located at $q_{\max} = \omega_0^2/a$ with energy $E_{\max} \equiv \Delta E = \omega_0^6/(6a^2)$. The Hamiltonian of the one-dimensional coupled nonlinear oscillator chain is given by

$$H = \sum_{n=1}^{N} \left\{ \frac{p_n^2}{2} + U(q_n) \right\} + \frac{\kappa}{2} \sum_{n=1}^{N} \left[q_{n+1} - q_n \right]^2 . \tag{2}$$

The coordinate q_n quantifies the displacement of the n-th oscillator in the local potential $U(q_n)$ (see Fig. 1) and p_n denotes the corresponding canonically conjugate momentum. The oscillators, also referred to as units, are coupled linearly to their neighbors with interaction strength κ.

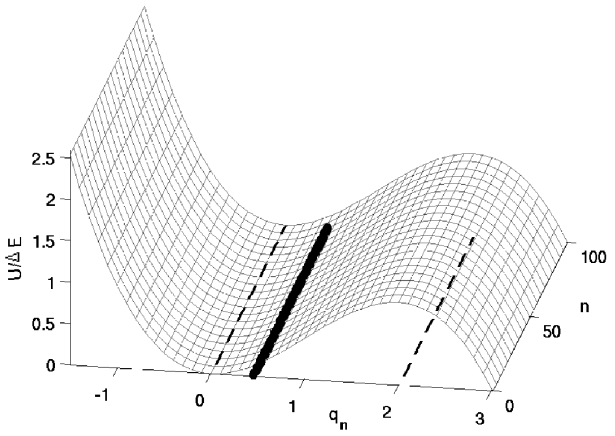

Fig. 1. Potential barrier with a chain positioned close to the bottom. The parameter values are $a = 1$, $\omega_0^2 = 2$, and $N = 100$.

The equations of motion derived from the Hamiltonian given in Eq. (2) read

$$\ddot{q}_n + \omega_0^2 q_n - a q_n^2 - \kappa \left[q_{n+1} + q_{n-1} - 2q_n \right] = 0 . \tag{3}$$

Periodic boundary conditions according to $q_{N+1} = q_1$ are employed. The total energy is conserved, *i.e.*, $E_{\text{total}} = \text{const}$. Notice, that the motion proceeds perpendicular to the axis of the one-dimensional chain and thus the appearance of a Goldstone mode is excluded.

3. Energy sharing and formation of arrays of breathers

In order to enhance the energy localization in the dynamics (3) with the potential (1) we propose the following scenario: on the average, an amount of energy $E_0 = E_{\text{total}}/N$ is applied per unit which allows the activation of

nonlinear, cooperative excitations of the chain. Thus, the chain possesses a total energy $E_{\text{total}} = \sum_{n=1}^{N} E_n = NE_0$. For an escape to take place we must require that $E_{\text{total}} > E_{\text{crit}} > \Delta E$. These inequalities convey the fact that more than just one unit governs the escape mechanism. The initial energy E_0 is supplied as follows: *(i)* First, the whole chain is placed at a fixed position $q_n(0) = q_0\,, \forall n\,$, near the bottom of the potential well. *(ii)* Then, the position of all units are iso-energetically randomized while keeping the total energy a constant — *i.e.*, $E_{\text{total}} = NE_0 = \text{const}$.

The random position values are uniformly distributed in an interval $|q_n(0) - q_0| \leqslant \Delta q$. The initial momenta are zero, *i.e.*, $p_n(0) = 0$. The mean values of q_0 are taken in such a way that the average excitation energy of a single oscillator, E_0, is small compared to the depth, ΔE, of the potential well. Due to the choice of sufficiently small detunings Δq the initial lattice state, $q_n(0) = q_0 + \Delta q_n$, is close to an almost homogeneous state and yet such disturbed that there result very small — but non-vanishing — initial interaction terms. More precisely, Eq. (4) determines the energy of a particle

$$E_n = \frac{p_n^2}{2} + U(q_n) + \frac{\kappa}{4}\left[(q_{n+1} - q_n)^2 + (q_{n-1} - q_n)^2\right]\,. \tag{4}$$

The last term in Eq. (4), representing the interaction energy of an individual particle, is typically of the order of $10^{-6} \times E_0$. Thus an energy exchange between the coupled units is entailed. The initial energy per unit obeys $E_0 \ll \Delta E$, but is still sufficiently large to initiate the excitation of nonlinear modes.

In this realm the formation of localized excitations can be explained by modulational instability [27–30]. This mechanism initiates an instability of a plane wave when small perturbations of non-vanishing wavenumbers are imposed. The instability — giving rise to an exponential growth of the perturbation — destroys the initial wave at a critical wavenumber. Eventually a pattern of localized humps gets formed, virtually with equal distance between them distributed on the chain [15–17]. A detailed study of the parameter's influences on the creation of the localized humps and in consequence on the escape process can be found in [17].

Finally we comment that in cases that the energy is supplied solely through the momenta, the energy localization scenario persists.

Regarding the initiation of the energy exchange we note that for small-amplitude solutions, $q_0 \simeq q_{\min}$, the anharmonic term in Eq. (2) is negligible. In an early stage of the dynamics the degree of energy exchange in dependence of the degree of detuning Δq can be estimated as follows:

Passing to action-angle variables

$$p_n = \sqrt{2\omega_0 J_n}\cos\theta_n\,, \qquad q_n = \sqrt{\frac{2J_n}{\omega_0}}\sin\theta_n\,, \tag{5}$$

the Hamiltonian (2) is expressed as

$$H = \sum_{n=1}^{N}\omega_0 J_n + \frac{\kappa}{2}\sum_{n=1}^{N}\left[\sqrt{\frac{2J_{n+1}}{\omega_0}}\sin\theta_{n+1} - \sqrt{\frac{2J_n}{\omega_0}}\sin\theta_n\right]^2 . \tag{6}$$

The evolution of the actions is determined by

$$\begin{aligned}\dot{J}_n = \quad & -\frac{\partial H}{\partial\theta_n} = \kappa\frac{2}{\omega_0}\sqrt{J_n}\cos\theta_n\Big[\sqrt{J_{n+1}}\sin\theta_{n+1} \\ & +\sqrt{J_{n-1}}\sin\theta_{n-1} - 2\sqrt{J_n}\sin\theta_n\Big]\,. \end{aligned}\tag{7}$$

Taking into account that for sufficiently small coupling κ action variables evolve much slower than angle variables [31] the evolution of the phase variables can be expressed as $\theta_n(t) = \omega_0 t + \theta_n^0$. With respect to our chosen initial conditions we set $\theta_n^0 = \pi/2$. The change in action during a time interval ΔT is given by

$$\begin{aligned}\delta J_n = \quad & \kappa\int_0^{\Delta T} dt\frac{2}{\omega_0}\sqrt{J_n}\cos(\omega_0 t + \pi/2) \\ & \times\left[\sqrt{J_{n+1}} + \sqrt{J_{n-1}} - 2\sqrt{J_n}\right]\sin(\omega_0 t + \pi/2) \\ = \quad & -\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)\sqrt{J_n}\left[\sqrt{J_{n+1}} + \sqrt{J_{n-1}} - 2\sqrt{J_n}\right]\,. \end{aligned}\tag{8}$$

Since the initial values of the coordinates are randomly distributed according to $|q_n(0) - q_0| \leqslant \Delta q$, the initial actions are correspondingly distributed as $|J_n(0) - J_0| \leqslant \Delta J$. We get the following estimate for the change in action during the interval ΔT:

$$\begin{aligned}|\delta J_n| \leqslant \quad & 2\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)\sqrt{J_0 + \Delta J}\left|\sqrt{J_0 + \Delta J} - \sqrt{J_0 - \Delta J}\right| \\ = \quad & 2\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)J_0\sqrt{1 + \Delta J/J_0}\left|\sqrt{1 + \Delta J/J_0} - \sqrt{1 - \Delta J/J_0}\right| \\ \approxeq \quad & 2\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)J_0\left(1+\frac{1}{2}\Delta J/J_0\right)\left|\left(1+\frac{1}{2}\Delta J/J_0\right) - \left(1-\frac{1}{2}\Delta J/J_0\right)\right| \\ = \quad & 2\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)\Delta J + O(\Delta J^2)\,. \end{aligned}\tag{9}$$

The actions stay close to their initial values if

$$\frac{\langle|\delta J|\rangle}{\langle J\rangle} \ll 1\,, \tag{10}$$

where $\langle\,\rangle$ denotes the spatial summation. We get

$$\langle J\rangle = \sum_{n=1}^{N} J_n \geqslant \sum_{n=1}^{N}(J_0 - \Delta J) = N(J_0 - \Delta J)\,, \tag{11}$$

and

$$\langle|\delta J|\rangle = \sum_{n=1}^{N} |\delta J_n| = 2N\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)\Delta J\,, \tag{12}$$

so that we finally obtain

$$\begin{aligned}\frac{\langle|\delta J|\rangle}{\langle J\rangle} &\leqslant 2\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)\Delta J/(J_0 - \Delta J)\\ &= 2\frac{\kappa}{\omega_0^2}\sin^2(\omega_0\Delta T)\Delta J/J_0 + O(\Delta J^2)\,.\end{aligned} \tag{13}$$

From this expression we infer that the rate of energy exchange vanishes for $\Delta J = 0$, and in reverse, increases with enlarging ΔJ expediting the energy exchange process.

To investigate the formation of intrinsically localized modes in our discrete system, the set of coupled Eqs. (3) has been numerically integrated with a fourth-order symplectic integrator scheme [32]. The accuracy of the calculation was checked by monitoring the conservation of the total energy with precision of at least $|(E(t) - E(0))/E(0)| = 10^{-9}$.

In agreement with our results above, we observe that starting from an early homogeneous state with an approximate equipartition of energy among all units the attainment of an array of breathers proceeds the faster the larger the width ΔJ respectively Δq . More precisely, due to the emergence of a modulational instability a pattern evolves in the course of time (of the order of $t \sim 10^3$) where for some lattice sites the amplitudes grow considerably remaining small in the adjacent regions. This feature is shown in Fig. 2 depicting the spatio-temporal evolution of the energy density, *cf.* (4).

Upon moving, these breathers tend to collide inelastically with others. In fact, various breathers merge to form larger amplitude breathers, proceeding preferably such that the larger amplitude breathers grow on the expense of the smaller ones. As a result, a certain amount of the total energy becomes strongly concentrated within confined regions of the chain. This localization scenario is characteristic for nonlinear lattice systems [33–41].

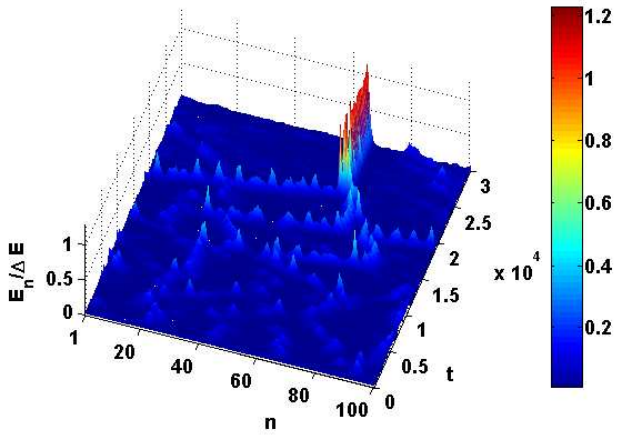

Fig. 2. (Color online) Spatio-temporal evolution of the energy density $E_n(t)$. The initial average energy per oscillator is only $E_0/\Delta E = 0.028$. The parameter values are $a = 1$, $\omega_0^2 = 2$, $\kappa = 0.2$, and $N = 100$.

4. Escape as the result of diffusion in a separatrix layer

In the last section we found that arrays of breathers form on the lattice. At least one of the breathers can be very strongly localized on segments of the lattice (single-site breathers) and the associated maximal amplitudes grow to the proximity of the barrier level. Moreover, in [15–17] it was shown that such a localized state might adopt the hairpin shape of the critical localized mode and if the involved amplitudes become overcritical escape is realized. However, for this to happen at first one unit has to absorb sufficient energy to completely surmount the barrier.

The escape process is based on energy redistribution produced by chaotic motion in the vicinity of a separatrix. To gain insight into the related energy diffusion process, we regard a segment of the lattice of odd numbers of sites N_s that sustains a single-site breather as decoupled from the rest of the lattice. The dynamics on the segment can be approximated by the motion of one of the oscillators with large amplitude near the separatrix. This oscillator is supposed to be situated at the central site of the segment denoted by n_c. The remaining $(N_\mathrm{s} - 1)/2$ units on either side of it perform oscillations near the bottom of the potential well, representing thus phonons. The corresponding Hamiltonian is expressed as

$$H = H_0 + H_1 \,, \tag{14}$$

with

$$H_0 = \frac{p_{n_\mathrm{c}}^2}{2} + \frac{\omega_0^2}{2} q_{n_\mathrm{c}}^2 - \frac{a}{3} q_{n_\mathrm{c}}^3 \,, \tag{15}$$

$$H_1 = \sum_{\substack{n=1 \\ n\neq n_\mathrm{c}}}^{N_\mathrm{s}} \left(\frac{p_n^2}{2} + \frac{\omega_0^2}{2} q_n^2 \right) + \frac{\kappa}{2} \sum_{n=1}^{N_\mathrm{s}} \left[q_{n+1} - q_n \right]^2 . \tag{16}$$

Here we assume sufficiently small κ so that H_1 acts as a small nonintegrable perturbation on the integrable motion associated with H_0.

That the central oscillator can overcome the potential barrier is connected with motion near a separatrix that is attributed to the hyperbolic equilibrium point in the corresponding p_{n_c}–q_{n_c}-plane. With the shift $q \to q - q_\mathrm{max}$ the hyperbolic point is located at the phase plane origin $(p, q) = (0, 0)$. For an isolated nonlinear oscillator the expression for the coordinate of the unperturbed separatrix solution is found as

$$q^s(t) \;=\; -\frac{3}{2} q_\mathrm{max} \,\mathrm{sech}^2 \left[\omega_0 (t - t_0)/2 \right] , \qquad -\frac{3}{2} q_\mathrm{max} \leq q \leq 0 , \tag{17}$$

$$q^s(t) \;=\; \frac{3}{2} q_\mathrm{max} \,\mathrm{cosech}^2 \left[\omega_0 (t - t_0)/2 \right] , \qquad q > 0 , \tag{18}$$

where t_0 determines the (initial) position on the separatrix. Expressions (17) and (18) are referred to as the left and right branch of the separatrix, respectively. The perturbation terms derived from H_1 cause the formation of a stochastic layer around the separatrix [31, 42]. The diffusive $p_{n_\mathrm{c}} - q_{n_\mathrm{c}}$−motion within the stochastic separatrix layer is driven by the neighboring small-amplitude oscillators. The total time rate of change of the energy $H_0 \equiv E_{n_\mathrm{c}}$ is determined by

$$\frac{dH_0}{dt} = \{H_0, H\} + \frac{\partial H_0}{\partial t} = -p_{n_\mathrm{c}} \, \kappa \, \left[q_{n_\mathrm{c}+1} + q_{n_\mathrm{c}-1} - 2 q_{n_\mathrm{c}} \right] . \tag{19}$$

The change during one ‘period’ of the separatrix motion is

$$\Delta H_0 = \int_{-\infty}^{\infty} dt \frac{dH_0}{dt} = -\kappa \int_{-\infty}^{\infty} dt \, \dot{q}^s_{n_\mathrm{c}} \left[q_{n_\mathrm{c}+1} + q_{n_\mathrm{c}-1} - 2 q^s_{n_\mathrm{c}} \right] . \tag{20}$$

For sufficiently small coupling κ we can express the evolution of the small-amplitude oscillators at sites $n_\mathrm{c} \pm 1$ as

$$q_{n_\mathrm{c}\pm1}(t) = q^0_{n_\mathrm{c}\pm1} \, \sin(\omega_0 t + \theta^0_{n_\mathrm{c}\pm1}) , \tag{21}$$

with $q^0_{n_\mathrm{c}\pm1}$ and $\theta^0_{n_\mathrm{c}\pm1}$ being the frozen amplitude and initial phase, respectively. Substituting (17) and (21) into (20), using the addition theorems for trigonometric functions, integrating once by parts and omitting the odd contributions to the integrand we obtain for the energy exchange

$$\Delta H_0 = 3 q_\mathrm{max} \kappa \sum_{\pm} q_{n_\mathrm{c}\pm1} \cos(\omega_0 t_0 + \theta^0_{n_\mathrm{c}\pm1}) \int_{-\infty}^{\infty} dt \, \mathrm{sech}^2(t) \cos(2t) . \tag{22}$$

Evaluating the integral one gets finally

$$\Delta H_0 = \frac{6\,\pi}{\sinh(\pi)} q_{\max} \kappa \sum_{\pm} q^0_{n_c \pm 1} \cos(\omega_0 t_0 + \theta^0_{n_c \pm 1})\,. \tag{23}$$

Notice that the expression (23) relates the local properties of the dynamics near the bottom (phonons) and barrier (breather amplitude) of the potential. We infer from (23) that the more the position of the saddle point is shifted to the right — *i.e.*, the larger $q_{\max}$, or in other words the ratio between the harmonicity and the anharmonicity strength ω_0^2/a, the higher is the energy exchange rate. In addition, the energy exchange rate (and the width of the stochastic layer) is proportional to the coupling strength and the phonon amplitudes. More importantly, it might be critically affected by the phase relation between the phonons at sites $n_c + 1$ and $n_c - 1$. Assuming symmetric patterns with $q^0_{n_c+1} = q^0_{n_c-1}$, we conclude that for overall in-phase motion $\theta^0_{n_c \pm 1} = \theta^0$ of the oscillators the stochastic separatrix layer is of maximal width. On the other hand, phase mismatches reduce the energy exchange rate (and the width of the stochastic separatrix layer). Therefore the region of unbounded motion extending along the right branch of the unstable manifold becomes only accessible to overcritically large breathing amplitudes that are very close to the separatrix level and otherwise overcoming the barrier is less likely. Finally, for out-of-phase motion $\theta^0_{n_c+1} = \theta^0_{n_c-1} \pm \pi$ the layer even vanishes.

The diffusion of the large amplitude oscillator in the separatrix layer driven by its adjacent oscillators is illustrated in Fig. 3. Prior to escape the corresponding phase curve (labeled n_c) meanders in the vicinity of the separatrix around which there is a stochastic layer (not shown in the figure). Once the trajectory has become captured by the right branch of the unstable manifold of the hyperbolic equilibrium point the motion proceeds afterwards in the direction of monotonically growing amplitude. From the moment the escaping unit has traveled beyond the hyperbolic point the phase curves of its neighbors (labeled $n_c \pm 1$) are superimposed on the plot. The adjacent units get dragged from the inside of the separatrix loop in the direction of the right branch of the unstable manifold. Consequently an escape of the entire chain is initiated.

Finally, we remark that the currently discussed escape process exhibits indeed some similarities with the corresponding process in the Kramers problem [1, 2] despite the presence of damping in the corresponding Langevin equation. In both cases, a unit, in order to escape from a potential well, has to overcome a barrier. Crucially, in contrast to the Kramers problem, the conservative — by far faster — escape process is self-induced by the internal irregular coupled dynamics and no other source like a heat bath is needed.

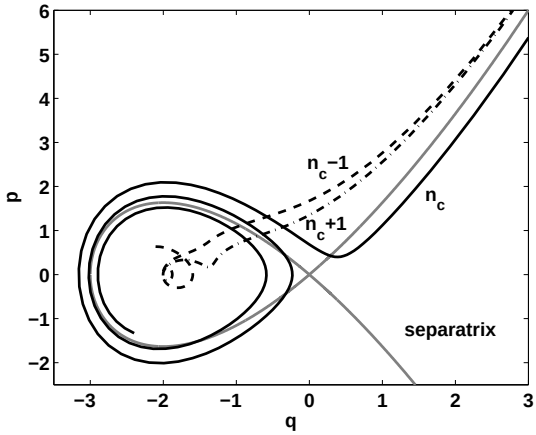

Fig. 3. Escape dynamics in the p–q-phase plane. Assignment of the line types as follows: solid gray line, unperturbed separatrix; solid black line, unit $n = n_{\mathrm{c}}$; dashed line, unit $n = n_{\mathrm{c}} - 1$; and dashed dotted line, unit $n = n_{\mathrm{c}} + 1$. Average initial energy per unit $E_0/\Delta E = 0.156$. The parameter values are $a = 1$, $\omega_0^2 = 2$, $\kappa = 0.2$, and $N = 100$. The coordinates are chosen such that the position of the saddle point comes to lie at the origin of the phase plane.

5. Summary

In this paper we have considered the conservative and deterministic dynamics of a one-dimensional chain consisting of linearly coupled anharmonic oscillators. Each oscillator evolves in a single well potential. Initially the system is in a metastable state for which all units are trapped near the bottom of the potential. Then overcoming of the barrier of the whole chain at once is prevented because of the too high net barrier height. In [15–17] it has been demonstrated, that the spontaneous formation of localized modes serves to enrich energetically a segment on the chain such advantageously that it adopts the transition state given in the form of a hairpin. Within this work we estimated the degree of energy exchange in an early stage of the dynamics. It turns out that the rate of energy exchange is crucially affected by the degree of detuning of the initial virtually homogeneous lattice state. Related to barrier crossing we presented the escape of the chain as the outcome of the diffusion process of a strongly localized breather amplitude in a separatrix layer. In particular it is shown that proper phase relations between the oscillators of the "phonon bath", driving the diffusion, play a crucial role for enhanced escape.

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