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# BREATHER SELF-TRAPPING AND DELOCALIZATION IN 2D SYSTEM OF WEAKLY COUPLED NONLINEAR CHAINS

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**Abstract**

We present analytical and numerical studies of nonlinear localized short-wavelength excitations (breathers) in a system of parallel weakly coupled chains of nonlinear oscillators, which in particular can model dynamics of weakly coupled polymer chains in polymer crystals. Periodic transverse translation (wandering) of low-amplitude breather in a system of several, up to five, coupled nonlinear chains is described, and the dependence of the wandering period on the number of chains is analytically estimated and compared with numerical results. On-chain self-trapping of large-amplitude 1D breather and delocalization of the breather in 2D system of a large number of coupled nonlinear chains is described, in which the breather, initially excited in a given 1D chain, abruptly spreads its vibrational energy in the whole 2D system upon decreasing breather frequency or amplitude below the threshold one. The threshold breather frequency is above the cut off phonon frequency in 2D system, and the threshold breather amplitude scales as square root of the inter-chain coupling constant. Such delocalizing transition of discrete breather in 2D and 3D system of coupled nonlinear chains also has an analogy with delocalizing transition of Bose-Einstein condensates in 2D and 3D optical lattices. The analytical results are confirmed by computer simulations.

Keywords: breather, delocalization, coupled nonlinear chains.

## 1 Introduction

The interest in studying moving nonlinear excitations in solids (solitons, kink-solitons, intrinsic localized modes and breathers, etc.) is strongly motivated by the fact that they can contribute to the thermal and thermal-transport properties of the material. Nonlinear excitations can be created most easily in low-dimensional systems, namely in 1D and quasi-1D anharmonic systems [Zabusky and Kruskal,1965; Kosevich and Kovalev, 1974; Dolgov, 1986; Sievers and Takeno, 1988; Page, 1990; Kosevich, 1993a; Kosevich, 1993b; Kosevich, 1993c; Aubry, 1997; Flach and Willis, 1998]. Solitons as self-trapped vibrational states were recently experimentally observed in quasi-1D $\alpha-$helices in proteins [Edler et al., 2004]. Solitons and intrinsic localized modes were also described and observed in low-dimensional ferromagnets and antiferromagnets [Kosevich, Ivanov and Kovalev, 1990; Kalinikos, Kovshikov and Patton, 1998; Sato and Sievers, 2004]. Polymer crystals, which consist of coupled long molecular chains, can be considered as an important example of quasi-1D solid-state structures. Kink-solitons and breathers were described in strongly anisotropic quasi-1D polymer crystals [Yakushevich, Savin and Manevitch, 2002; Savin and Manevitch, 2003; Savin, Zubova and Manevitch, 2005]. In optics, a single or coupled nonlinear wavequides present another example of experimentally accessable and technologically important quasi-1D systems [Hasegawa, 1990; Eisenberg et al., 1998; Peschel et al., 1999]. One-dimensional arrays of magnetic or optical microtraps for Bose-Einstein condensates of ultracold quantum gases with tunneling coupling between them provide yet another new field for the studies of nonlinear coherent dynamics in low-dimensional systems [Anderson and Kasevich, 1998; Trombettoni and Smerzi, 2001; Anker et al., 2005].

On the other hand, the mechanical or tunneling coupling between quasi-1D systems can result in a variety of new nonlinear effects. Among them the beating (or wandering) of the nonlinear excitation between two or more coupled quasi-1D systems is an interesting and important phenomenon, which can be revealed in all of the aforementioned systems. Pulse switching in nonlinear fiber directional couplers [Uzunov et al., 1995; Valkering, van Honschoten and Hoekstra, 1999] and optical Bloch oscillations in wavequide arrays [Pertsch et al., 1999] can be mentioned as examples of the beating phenomena in optical waveguides. A dynamical transition from Josephson oscillations to nonlinear self-trapping, which was recently observed in a single bosonic Josephson junction between two Bose-Einstein condensates [Albiez et al., 2005], is another fascinating example of the nonlinear beating phenomenon.

In our recent work, we have performed analytical and numerical studies of nonlinear localized short-wavelength excitations (breathers) in a system of two weakly coupled chains of nonlinear oscillators [Kosevich, Savin and Manevitch, 2007]. We have shown that after the initiation of a breather on one of the two coupled chains, under certain initial conditions it can gradually transfer to another chain and then return back ($wandering\ breather$). A separatrix between the wandering and on-chain-localized ($self$-$trapping$) regimes of breather dynamics in the two-chain system is described, at which the rate of energy exchange between the chains decreases drastically. In this paper we present analytical and numerical studies of nonlinear localized short-wavelength excitations (breathers) in a system of parallel weakly coupled chains of nonlinear oscillators, which in particular can model dynamics of weakly coupled polymer chains in polymer crystals. Periodic transverse translation (wandering) of low-amplitude breather in a system of several, up to five, coupled nonlinear chains is described, and the dependence of the wandering period on the number of chains is analytically estimated and compared with numerical results. On-chain self-trapping of large-amplitude 1D breather and delocalization of the breather in 2D system of a large number of coupled nonlinear chains is described, in which the breather, initially excited in a given 1D chain, abruptly spreads its vibrational energy in the whole 2D system upon decreasing breather frequency or amplitude below the threshold one. The threshold breather frequency is above the cut off phonon frequency in 2D system, and the threshold breather amplitude scales as square root of the inter-chain coupling constant. Such delocalizing transition of discrete breather in 2D and 3D system of coupled nonlinear chains also has an analogy with delocalizing transition for polarons in 2D and 3D lattices [Kalosakas, Aubry and Tsironis, 1998] and for Bose-Einstein condensates in 2D and 3D optical lattices [Kalosakas, Rasmussen and Bishop, 2002]. The analytical results are confirmed by computer simulations.

## 2 Analytical model and numerical simulation

Quasi-1D system of $M$ parallel weakly coupled anharmonic chains, with unit intra-chain period and inter-chain spacing, with nearest-neighbor intra- and inter-chain interactions, is described by the following Fermi-Pasta-Ulam (FPU) Hamiltonian:

$$H = \sum_{m=1}^{M}\sum_{n=1}^{N}\frac{1}{2}\dot{u}_{m,n}^2 + \sum_{m=1}^{M}\sum_{n=1}^{N-1}V(u_{m,n+1}-u_{m,n}) + \sum_{m=1}^{M-1}\sum_{n=1}^{N}U(u_{m+1,n}-u_{m,n}), \quad (1)$$

where $n = 1, ..., N$ and $m = 1, ..., M$ numerate, respectively, sites along the chains and chains, and

$$V(x) = \frac{1}{2}x^2 + \frac{1}{3}\alpha x^3 + \frac{1}{4}\beta x^4, \quad (2)$$

$$U(x) = \frac{1}{2}Cx^2. \quad (3)$$

with $C = 0.1$ describing the strength of the weak inter-chain coupling.

In Eq. (1) $u_n^{(i)}$ is displacement of the $n$-th particle from its equilibrium position in the $i$-th chain, $p_n^{(i)} = \dot{u}_n^{(i)}$ is particle momentum, $\alpha^{(i)}$, $\beta^{(i)}$ and $C$ are, respectively, intra-chain linear, intra-chain nonlinear and inter-chain linear force constants. We assume that the coupling is weak, $C = 0.1$, and therefore do not include the nonlinear inter-chain interaction. The $\beta$-FPU Hamiltonian (1) (with $\alpha = 0$) describes, e.g., purely transverse particle motion [Kosevich, 1993b]. Torsion dynamics of DNA double helix can also be approximated by the $\beta$-FPU Hamiltonian (1) [Yakushevich, Savin and Manevitch, 2002]. On the other hand, weakly coupled nonlinear molecular chains in polymers are characterized by the asymmetric intra-chain anharmonic potential, with nonzero $\alpha^{(i)}$ [Savin and Manevitch, 2003; Savin, Zubova and Manevitch, 2005].

Hamiltonian (1) generates corresponding equations of motion,

$$\ddot{u}_{m,n} = -\frac{\partial H}{\partial u_{m,n}}, \quad (4)$$

which in the linear approximation have the form:

$$\ddot{u}_{m,n} = u_{m,n+1} - 2u_{m,n} + u_{m,n-1} + C(u_{m+1,n} - 2u_{m,n} + u_{m-1,n}). \quad (5)$$

Plane linear waves (phonons) in such system, with

$$u_{m,n} = u\exp[iq_1 n + iq_2 m - i\omega t], \quad (6)$$

have the dispersion:

$$\omega(q_1, q_2) = \sqrt{2[1-\cos q_1 + C(1-\cos q_2)]}, \quad (7)$$

where both the intra-chain lattice period and inter-chain spacing are taken equal to unit, and therefore $0 \leq (q_1, q_2) \leq \pi$. Minimal phonon frequency in this translationally-invariant system is zero, $\omega(0,0) = 0$, while cut off phonon frequency is $\omega(\pi,\pi) = 2\sqrt{1+C}$ (which is equal to $\omega(\pi,\pi) = 2.0976 \approx 2.1$ for $C = 0.1$).

Since we will be interested in the short-wavelength excitations, with $q_1 \approx \pi$, the corresponding phonon frequency for $C \ll 1$,

$$\omega(q_1 \approx \pi, q_2) = 2 + C\sin^2(\frac{1}{2}q_2), \qquad (8)$$

determines the phonon group velocity across the chains:

$$V_\perp(q_1 \approx \pi, q_2) = \frac{\partial\omega(q_1 \approx \pi, q_2)}{\partial q_2} = \frac{1}{2}C\sin(q_2). \qquad (9)$$

Now we turn to the nonlinear dynamics of $M$ weakly coupled parallel nonlinear chains with Hamiltonian (1). We will integrate Eqs. (4) with the initial condition which describes exact discrete breather in the $m$-th chain ($1 \le m \le M$) under the condition of immovability of the rest of the chains, to study the time dependence (for $t > 0$) of the vibrational energy in the chains:

$$E_m = \frac{1}{2}\sum_{n=1}^{N}(\dot{u}^2_{m,n} + V_{m,n} + V_{m,n-1} + U_{m,n} + U_{m-1,n}), \qquad (10)$$

where $V_{m,n} = V(u_{m,n+1} - u_{m,n})$, $U_{m,n} = U(u_{m+1,n} - u_{m,n})$.

In Figs. 1 (a,b,c,d) we show the time dependence of energies of the first, $i = 1$, and the last, $i = M$, coupled chains for $M = 2, 3, 4, 5$, for the time interval just after breather excitation on the first chain, left panel, and for the later time, right panel. In the case of $M = 2$, there is a periodic (harmonic) complete energy exchange between the first and the second chains, see Fig. 1(a). In the case of $M = 3$, there is periodic (non-harmonic) recurrence of the complete energy accumulation in the first chain, and the period of such recurrence is twice larger (the recurrence rate is twice smaller) than that in the case of $M = 2$. The time dependence of the first chain energy recurrence can be roughly approximated by $\cos^4(Ct/8)$ (instead of $\cos^2\Theta = \cos^2(Ct/4)$ in the case of $M = 2$, see Ref. [Kosevich, Savin and Manevitch, 2007], similar to the time dependence of the population of the initially excited state in a three-state (spin 1) atomic system, see, e.g., Ref. [Mewes et al., 1997]. Here $C/4$ plays role of the Rabi frequency, which is twice smaller than the rate of the complete energy exchange (energy recurrence) in the case of $M = 2$, when it is equal to $C/2$. In the case of $M = 4$ and $M = 5$, the recurrence of energy of the first (and the last chain) becomes quasi-periodic, but still the (approximate) period $T_M$ of such recurrence scales with the number of chains $M$ as $T_M \propto (M-1)$. For $M \ge 6$, $C = 0.1$, the initially localized (in chain 1) excitation spreads its energy in the whole system of weakly coupled chains.

The dependence of the recurrence period $T_M$ on $M$ we can relate with the transverse group velocity, Eq. (9), of the high-frequency phonons (with $q_1 \approx \pi$) in the system of weakly coupled anharmonic chains. The transverse wavevector $q_2$ in Eq. (9) is equivalent to the relative phase of the neighboring chains. In the regime of almost-harmonic energy transfer between the neighboring chains, the relative phase is always close to $\pi/2$, see Fig. 1. It means that the transverse wavevector $q_2$ in the expression (9) for the transverse group velocity of the wandering breather should also be (approximately) equal to $\pi/2$. This gives $V_\perp \approx \frac{1}{2}C$ for this velocity. Essentially this characteristic group velocity does not depend on the number of the coupled chains $M$. Therefore we can estimate the period of the first chain energy recurrence as $T_M = 2B(M-1)/V_\perp \approx 4B(M-1)/C$ with some dimensionless factor $B$, which is consistent with our numerical observation (with $B \approx 3$).

The same transverse phonon group velocity one can estimate from Fig. 2 as the speed of breather spreading across the chains. Figure 2 shows the time dependence of energy distribution among the chains when breather was initially excited in the edge chain, Figs. 2(a) and 2(b), or in the central chain, Figs. 2(c) and 2(d), in the system of $M = 50$ coupled chains. As follows from Figures 2(a) and 2(c), the initial-breather energy has spread for 20 chains for approximately 500 time units. This gives us quantitative estimate of 0.04 for the transverse group velocity, which is rather close to our analytical estimate with the use of Eq. (9) for $q_2 \approx \pi/2$: $V_\perp \approx \frac{1}{2}C = 0.05$. Figure 2 also shows that the appearance of localized breather in a system of coupled chains, with $M \gg 2$, has a threshold in breather frequency, $\omega_{thresh} = 2.15$ in Fig. 2(b) and $\omega_{thresh} = 2.17$ in Fig. 2(d),t similar to the case of two coupled chains [Kosevich, Savin and Manevitch, 2007]. The minimal breather frequency, which corresponds to the appearance of localized breather in a system of coupled chains, we should compare with breather frequency at the separatrix in a system of two coupled chains, $\omega_{sep} \approx 2.1$ for $C = 0.1$ and $\alpha = 0$, see Ref. [Kosevich, Savin and Manevitch, 2007]. Since all the above frequencies are close, we can get the estimate for the threshold breather amplitude for its localization in 2D system of weakly coupled chains: $\Psi^{thresh}_{max} \sim \sqrt{C/\beta}$. For $\Psi_{max} < \Psi^{thresh}_{max}$, the 1D breather, which was initially excited in one chain, will start to translate laterally to the neighboring chains, will spread its energy among them and lose it due to phonon emission, and finally will decay into small-amplitude phonons due to lowering of its frequency up to the cut off phonon frequency $\omega_{max} = 2\sqrt{1+C}$, see Figs. 2(a) and 2(c). Such evolution of low-amplitude 1D breathers can also be related with the conclusion in Ref. [Kosevich, Savin and Manevitch, 2007] that wandering breather is not an exact solution of the nonlinear system even in the case of two coupled anharmonic chains. In contrast to this behavior of low-amplitude breathers, 1D breather with the amplitude $\Psi_{max} > \Psi^{thresh}_{max}$ is self-trapped and remains localized mainly in the chain of its initial excitation, see Figs. 2(b) and 2(d). [In Fig. 2(d) one can see a partial (incomplete) energy exchange between the central chain and its nearest neighbors, similar to the incomplete energy exchange in two coupled chains beyond the separatrix, cf. [Kosevich, Savin and Manevitch, 2007]]. This phenomenon resembles the so-called $delocalizing\ transition$ in 2D system, when the wave field abruptly changes its character from spatially localized to the extended one, cf. similar delocalizing transition for polarons in 2D and 3D lattices [Kalosakas, Aubry and Tsironis, 1998] and for Bose-Einstein condensate in 2D optical lattice [Kalosakas, Rasmussen and Bishop, 2002]. In our case, the delocalizing transition occurs by the decrease of the initial breather amplitude $\Psi_{max}$ (or frequency $\omega$) from the value $\Psi_{max} > \Psi_{max}^{thresh} \sim \sqrt{C/\beta}$ (or $\omega > \omega_{thresh}$) to the value $\Psi_{max} < \Psi_{max}^{thresh}$ (or $\omega < \omega_{thresh}$). Such transition is related with finite energy threshold for the creation of solitons and breathers in 2D and 3D systems, see Refs. [Kingsep, Rudakov and Sudan, 1973; Flach, Kladko and MacKay, 1997], and is absent in 1D ($\beta$-FPU or discrete nonlinear Schrödinger equation [Kalosakas, Aubry and Tsironis, 1998; Kalosakas, Rasmussen and Bishop, 2002]) systems. Indeed, the threshold breather amplitude $\Psi_{max}^{thresh}$ in strongly anisotropic quasi-1D system vanishes in the limit $C \to 0$ of a single 1D chain as $\Psi_{max}^{thresh} \sim \sqrt{C/\beta}$. Similar threshold breather amplitude $\Psi_{max}^{thresh} \sim \sqrt{C/\beta}$ for breather delocalization should also appear in 3D array of parallel weakly coupled, with coupling constant $C \ll 1$, nonlinear chains which are described by the FPU Hamiltonian, similar to the one given by Eq. (1).

## 3 Summary

We have shown that low-amplitude breather can perform periodic transverse translation (wandering) in a system of several, up to five, coupled nonlinear chains. The dependence of the wandering period on the number of chains is analytically estimated and compared with numerical results. We have also shown the on-chain self-trapping of large-amplitude 1D breather and delocalization of the breather in 2D system of a large number of coupled nonlinear chains. The delocalization occurs when the breather, initially excited in a given 1D chain, abruptly spreads its vibrational energy in the whole 2D system upon decreasing breather frequency or amplitude below the threshold one. The threshold breather frequency is above the cut off phonon frequency in 2D system, and the threshold breather amplitude scales as square root of the inter-chain coupling constant.

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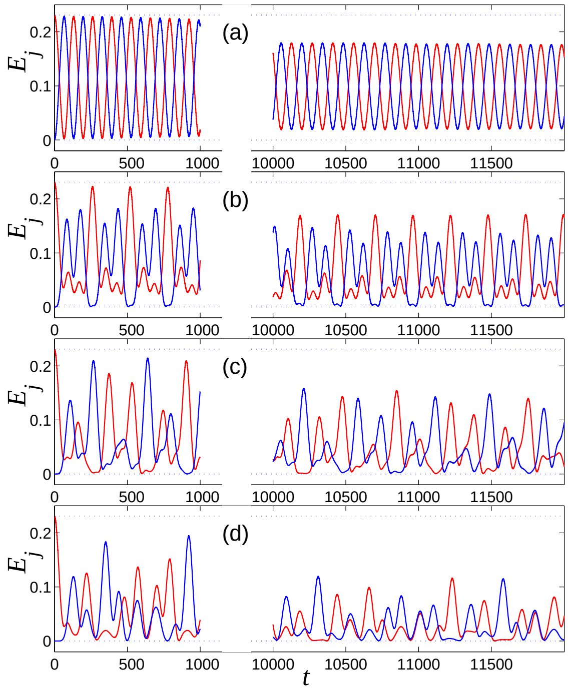


Figure 1. (color online) Time dependence of breather energy in first (red) and last (blue) chains in a system of 2 (a), 3 (b), 4 (c), and 5 (d) chains with $C = 0.1$, $\alpha = 0$, $\beta = 1$. The breather was initially excited with frequency $\omega = 2.05$ in chain 1, with immovable rest of the chains.

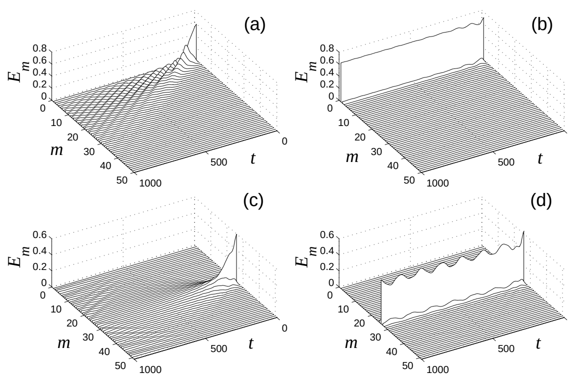


Figure 2. Time dependence of breather energy distribution between chains in a system of 50 coupled chains with $C = 0.1$, $\alpha = 0$, $\beta = 1$. Here $m$ is chain number and $E_m$ is energy of the $m$-th chain. The breather was initially excited (a) with frequency $\omega = 2.14$ in chain 1, (b) with frequency $\omega = 2.15$ in chain 1, (c) with frequency $\omega = 2.16$ in chain 25, (d) with frequency $\omega = 2.17$ in chain 25, with immovable rest of the chains.