Discrete breathers in vibroimpact chains: Analytic solutions

O. V. Gendelman[1,*] and L. I. Manevitch[2]
[1] *Faculty of Mechanical Engineering, Technion-Israel Institute of Technology, Haifa 32000, Israel*
[2] *Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia*

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We present exact analytic solutions for discrete breathers in essentially nonlinear oscillatory chains, belonging to both of the most common universality classes (Klein-Gordon and Fermi-Pasta-Ulam). The exact solutions can be obtained due to use of vibroimpact potentials, combining extreme nonlinearity with the possibility of description in terms of a forced linear model under conditions of self-consistency. A crossover between the cases of high and low energies can be studied directly. The solutions obtained may be used as a high-energy limit for models with other realistic potentials, as well as benchmarks for the testing of approximate approaches in the theory of discrete breathers.

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I. INTRODUCTION

Discrete breathers (DB), or spatially localized time-periodic solutions in Hamiltonian classic nonlinear lattices, were discovered in the late 1960s and have attracted a lot of attention [1–5]. These solutions appear both in Klein-Gordon (KG) lattices with nonlinear on-site potential [6] and in Fermi-Pasta-Ulam (FPU) lattices with nonlinear interaction between the particles [7,8]. For both types of models mentioned above, the DB have well-developed theory [3] and a wide range of applications, including Josephson contacts, nanomechanical systems, Bose-Einstein condensates, carbon nanotubes, etc. [3].

Despite all these developments, to the best of our knowledge there exist only two nontrivial models that allow exact computation of the DB. The first one is the well-known integrable Ablowitz-Ladik model [9], one of the discrete counterparts of the nonlinear Schrödinger equation. The other model was suggested by Ovchinnikov and Flach [10]. This model explores the DB in the lattices with homogeneous potentials. It should be mentioned that neither of these models belongs to the most common KG or FPU type.

The goal of this paper is to construct the exact solutions for discrete breathers in one-dimensional chains with a nonlinearity of impact type. The impact interaction has the strongest nonlinearity possible—its potential corresponds to a vertical wall. The models with impacts are widely used for simulation of various physical phenomena. Some examples are various types of billiards [11,12], the model of a bouncing ball leading to the celebrated standard map in the theory of chaos [13,14] or models involving colliding particles, which are explored in connection with fundamentals of heat conduction [15–17]. Of course, this list is far from being exhaustive.

The models considered in this paper also involve elastic collisions, but the latter are combined with common linear elastic interactions. Such combined models are widely studied in some branches of theory of vibrations and mechanical engineering [18,19], but have only limited use in relation to physical phenomena (although some applications do exist; see, e.g., [20]).

*Author to whom correspondence should be addressed: ovgend@tx.technion.ac.il

II. DESCRIPTION OF THE MODEL AND ANALYTIC TREATMENT

A. System of Klein-Gordon (KG) type

Let us consider a one-dimensional linear chain with every particle placed between on-site impact barriers. The equations of motion are

$$\ddot{u}_n + c(2u_n - u_{n-1} - u_{n+1}) = 0, \quad |u_n| < \Delta, \tag{1}$$

$$n = 0, \pm 1, \pm 2, \dots .$$

Scalar u_n denotes the displacement of the nth particle, the mass of each particle is adopted to be unit, and c is the rigidity of the linear coupling. The distance between the barriers at each site is equal to 2Δ. An interaction of every particle with the barrier as the displacement achieves $\pm\Delta$ is described as a purely elastic impact. This means that if the impact occurs at time t_0, then the following condition holds for all n:

$$\lim_{t \to t_0 - 0} \dot{u}_n = - \lim_{t \to t_0 + 0} \dot{u}_n \big|_{u_n = \pm\Delta}. \tag{2}$$

System (1) can be considered as particular case of discrete Klein-Gordon lattices. It should be stressed that system (1) is homogeneous, i.e., the impact barriers exist at every site. System (1) is obviously nonintegrable; still, we are going to demonstrate that due to its simplicity, it is possible to obtain exact solutions for the DB.

Let us look for the solution of Eqs. (1) and (2) with only one particle subject to periodic impacts with the barriers. Without loss of generality, we suggest that it is particle $n = 0$. Such impacts are equivalent to the action of periodic external δ pulses on this particle. In other terms, for particular solutions we are seeking for system (1) and (2), they are equivalent to the following system of equations:

$$\ddot{u}_n + c(2u_n - u_{n-1} - u_{n+1}) = 2p\delta_{n0}\sum_{k=-\infty}^{\infty}[\delta(t - T/4 + kT) - \delta(t + T/4 + kT)], \tag{3}$$

where T is the period of the impacts, $2p$ is the unknown change of the particle moment in the course of the impact, and δ_{ij} is the Kronecker symbol.

At this point, the crucial advantage of the vibroimpact model reveals itself—Eq. (3) is linear and may be solved exactly. This possibility of simplification was used for computing the nonlinear normal modes in vibrating systems with impacts [21]. Once the solution is obtained, one should check whether it satisfies the following conditions of self-consistence:

(a) Maximal displacement of the particle $n=0$ is equal to Δ.

(b) Maximal displacements of all particles with $n \neq 0$ are less than Δ (no other impacts occur).

If both of these conditions are satisfied, then the solution of forced linear equation (3) is a genuine solution of initial system (1).

It is convenient to rewrite the right-hand side of Eq. (3) as Fourier series (in the sense of distributions),

$$\ddot{u}_n + c(2u_n - u_{n-1} - u_{n+1}) = \delta_{n0}\frac{4p\omega}{\pi}\sum_{j=1}^{\infty}(-1)^j \sin[(2j-1)\omega t]. \tag{4}$$

Here $\omega = 2\pi/T$. Thus, the conditions of the impact are equivalent to local forcing of the chain with multiple frequencies. The dispersion relation for traveling waves in the linear chain is well known,

$$\Omega^2 = 2c(1 - \cos q), \tag{5}$$

where Ω is the wave frequency and q is the wave number. Consequently, the frequency spectrum of any periodic localized solution must be situated in the attenuation zone, above the maximum frequency

$$\Omega_{max} = 2\sqrt{c}. \tag{6}$$

The forcing terms in Eq. (4) have frequencies ω, 3ω, 5ω, etc. Consequently, the forced solution of Eq. (4) will be localized if

$$\omega > \Omega_{max}. \tag{7}$$

Stationary solution of Eq. (4) may be easily found with the help of Z transform. It can be written down in the following form:

$$u_n(t) = \frac{(-1)^n p\omega}{\pi c}\sum_{j=1}^{\infty}(-1)^j \times \frac{[2\mu(2j-1)^2 - 1 - 2\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]^{|n|}}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}} \times \sin[(2j-1)\omega t],$$

$$\mu = \frac{\omega^2}{4c}. \tag{8}$$

Maximum displacement of the particle $n=0$ should be equal to the impact threshold Δ. It is achieved when $t=T/4+kT/2$. In other terms,

$$|u_0(T/4)| = \frac{p\omega}{\pi c}\sum_{j=1}^{\infty}\frac{1}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}} = \Delta. \tag{9}$$

From Eq. (9), one obtains the value of the unknown coefficient p. With account of Eq. (9), Eq. (8) is reduced to the following form:

$$u_n(t) = (-1)^n\Delta\frac{\sum_{j=1}^{\infty}(-1)^j\frac{[2\mu(2j-1)^2 - 1 - 2\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]^{|n|}}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}\sin[(2j-1)\omega t]}{\sum_{j=1}^{\infty}\frac{1}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}}. \tag{10}$$

Expression (10) is the exact solution for the DB in system (1) and (2). First of all, it should be mentioned that the series converge both in the numerator and in the denominator. In the numerator, the coefficients for Fourier series decay like $(2j-1)^{-(n+2)}$ for large j; in the same limit, the series in the denominator behaves like $\Sigma(2j-1)^{-2}$.

Maximum displacement of the nth particle is expressed as

$$|u_n(T/4)| = \Delta\frac{\sum_{j=1}^{\infty}\frac{[2\mu(2j-1)^2 - 1 - 2\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]^{|n|}}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}}{\sum_{j=1}^{\infty}\frac{1}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}}. \tag{11}$$

It is easy to demonstrate that the function

$$F(x) = 2x - 1 - 2\sqrt{x^2 - x} \tag{12}$$

for $x > 1$ obeys $1 > F(x) > 0$ and decreases monotonously when x grows. Thus, the following inequalities hold:

$$|u_n(T/4)| = \Delta \frac{\displaystyle\sum_{j=1}^{\infty} \frac{[2\mu(2j-1)^2 - 1 - 2\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]^{|n|}}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}}{\displaystyle\sum_{j=1}^{\infty} \frac{1}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}} < (2\mu - 1 - 2\sqrt{\mu^2 - \mu})^{|n|}\Delta = (2\mu - 1 - 2\sqrt{\mu^2 - \mu})^{|n|}|u_0(T/4)|. \tag{13}$$

If $\mu > 1$ (i.e., the basic frequency of the impacts ω is in the attenuation zone), then the solution (10) is exponentially localized, as one should expect for the DB. Besides, for any n the maximum displacement of the particles is less than Δ, i.e., they are not engaged in the impacts. This observation concludes the proof of consistency for solution (10).

It seems not possible to compute closed expressions for series in expression (10). Still, the series converge fast enough, so no special computation difficulties are encountered.

In order to illustrate the solution (10), we plot the breather profile—maximum displacement for each particle—for $\mu = 3$ [basic frequency far from the boundary of the attenuation zone, Fig. 1(a)] and $\mu = 1.05$ [basic frequency close to the boundary of the attenuation zone, Fig. 1(b)]. Δ is adopted to be unity. From obvious symmetry considerations, it is enough to plot only the particles with $n \geqslant 0$.

One can see that, as expected, the breather with basic frequency far from the boundary of the propagation zone is strongly localized, whereas the DB relatively close to this boundary is much wider. In order to assess the type of motion exhibited by different particles, it is instructive to plot the time dependence of displacement for $n = 0$ and 1 for the same values of Δ and μ as in Figs. 2(a) and 2(b).

One can see that for even a moderately high basic frequency of the DB (in the case $\mu = 3$, the frequency is only 1.73 of the gap value), the displacement of the particle $n = 0$ resembles the triangular wave and its shape is very different from $n = 1$. Quite obviously, the continuum approximation would be completely unsuitable for this case. Alternatively, close to the gap boundary, for $\mu = 1.05$ the "impact" part reveals itself only near the maximum.

In this connection, let us investigate the limit cases of solution (10). For the limit of high frequencies $\mu \to \infty$, one obtains

$$u_n(t) = \begin{cases} 0, & n \neq 0 \\ \dfrac{8\Delta}{\pi^2} \displaystyle\sum_{j=1}^{\infty} (-1)^j \frac{\sin[(2j-1)\omega t]}{(2j-1)^2}, & n = 0. \end{cases} \tag{14}$$

For $n = 0$, sum (14) indeed describes a triangle wave with frequency ω. This situation exactly corresponds to the "anti-integrability" limit well known in the theory of the DB [22], where the oscillations are concentrated on a single particle.

The other limit, $\mu \to 1$, physically corresponds to the close vicinity of the boundary of the attenuation zone. Let us consider the case

$$\mu = 1 + \varepsilon, \quad 0 < \varepsilon \ll 1. \tag{15}$$

For this case,

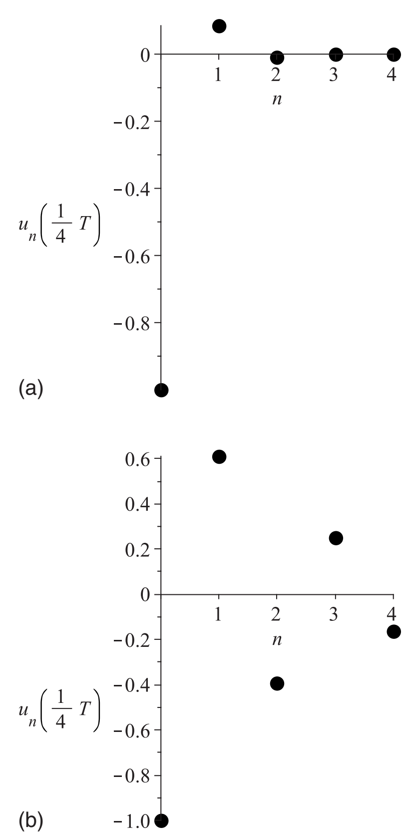

FIG. 1. Profile of the discrete breather (model of KG type). Maximum amplitudes of the particles are plotted: (a) $\mu = 3$, (b) $\mu = 1.05$.

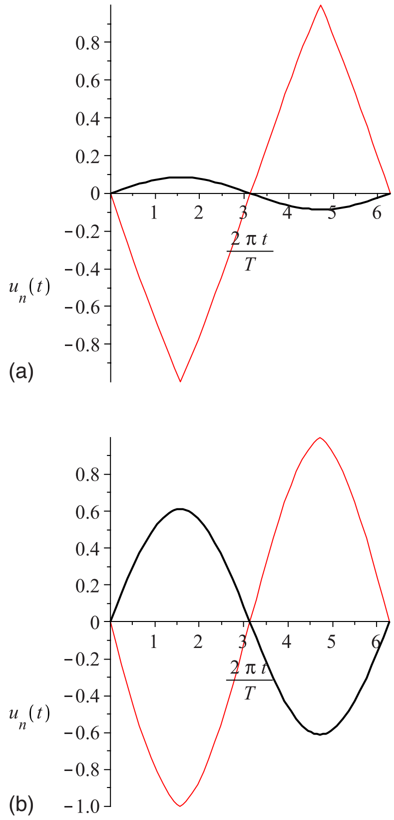

FIG. 2. (Color online) Time history of the particles in KG-type model: thin line, $u_0(t)$; thick line, $u_1(t)$; (a) $\mu=3$, (b) $\mu=1.05$.

$$\frac{1}{\sqrt{\mu^2(2j-1)^4-\mu(2j-1)^2}} = \begin{cases} \dfrac{1}{\sqrt{\varepsilon}}+O(\sqrt{\varepsilon}), & j=1 \\ \dfrac{1}{2(2j-1)\sqrt{j^2-j}}+O(\varepsilon), & j>1. \end{cases} \tag{16}$$

From estimation (16) it is clear that in the lowest order of approximation, only the term with $j=1$ should be kept in all sums in Eq. (10). Consequently, the approximate solution will read

$$u_n(t) = -(-1)^n\Delta(1-2\sqrt{\varepsilon})^{|n|}\sin\omega t + O(\sqrt{\varepsilon}), \quad \varepsilon\to 0. \tag{17}$$

Solutions of this type are obtained when the DB is rather widely searched as a solution of the continuous modulated system [23].

B. System of Fermi-Pasta-Ulam (FPU) type

The method for obtaining the exact DB solutions described above can be extended for a model with gradient nonlinearity without the on-site potential chain of the FPU type. If the potential of interaction between the neighboring particles is $V(u_n-u_{n-1})$, then the equations of motion will be

$$\ddot{u}_n + \frac{\partial V(u_n-u_{n-1})}{\partial u_n} + \frac{\partial V(u_{n+1}-u_n)}{\partial u_n} = 0. \tag{18}$$

In the symmetric vibroimpact model, the impacts occur when the displacement between the neighboring particles achieves a certain limit value (from above and from below). Thus, the potential $V(x)$ is defined as

$$V(x) = \frac{1}{2}cx^2, \quad |x|<D. \tag{19}$$

When the relative displacement achieves its limit value D at time t_0, the impact (actually, the pair of impacts) occurs and the relative velocity changes its sign. Similarly to Eq. (2), one can formulate this condition as

$$\lim_{t\to t_0-0}(\dot{u}_n-\dot{u}_{n-1}) = -\lim_{t\to t_0+0}(\dot{u}_n-\dot{u}_{n-1})\big|_{u_n-u_{n-1}=\pm D}, \tag{20}$$

$$n=0,\pm 1,\pm 2\ldots\ .$$

The simplest situation, which corresponds to the DB, will occur if only one interparticle bond will have elongations large enough to cause impacts. Without the loss of generality, let us suppose that this bond is one between the particles $n=0$ and 1. The action of impacts may be substituted by the action of two series of δ pulses, acting in opposite directions at the particles 0 and 1. Consequently, this particular solution will satisfy the following equations of the motion:

$$\ddot{u}_n + c(2u_n-u_{n-1}-u_{n+1}) = 2p(\delta_{n0}-\delta_{n1})\sum_{k=-\infty}^{\infty}[\delta(t-T/4+kT) - \delta(t+T/4+kT)]. \tag{21}$$

The left-hand side of Eq. (21) is linear and so there is no need to solve it once more—the solution can be obtained by appropriate superposition. Based on Eq. (8), the solution will be

$$u_n(t) = Q(n,t) - Q(n-1,t),$$

$$Q(n,t) = \frac{(-1)^n p\omega}{\pi c}\sum_{j=1}^{\infty}(-1)^j \times \frac{[2\mu(2j-1)^2-1-2\sqrt{\mu^2(2j-1)^4-\mu(2j-1)^2}]^{|n|}}{\sqrt{\mu^2(2j-1)^4-\mu(2j-1)^2}} \times \sin[(2j-1)\omega t]. \tag{22}$$

In order to determine the unknown coefficient p, one should normalize solution (22) according to the impact condition (20). By denoting the relative displacement,

$$w_n = u_{n+1}-u_n, \tag{23}$$

we get from Eq. (22),

$$w_0(t) = u_1(t) - u_0(t) = Q(-1,t) + Q(1,t) - 2Q(0,t)$$
$$= -\frac{4p\omega}{\pi c}\sum_{j=1}^{\infty}(-1)^j \times \frac{[\mu(2j-1)^2 - \sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}} \times \sin[(2j-1)\omega t]. \quad (24)$$

The normalization condition will then read

$$|w_0(T/4)| = \frac{4p\omega}{\pi c}\sum_{j=1}^{\infty}\frac{[\mu(2j-1)^2 - \sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}} = D. \quad (25)$$

Finally, the solution for the DB in the FPU-type vibroimpact chain will be

$$u_n(t) = Z(n,t) - Z(n-1,t),$$

$$Z(n,t) = \frac{(-1)^n D \sum_{j=1}^{\infty}(-1)^j \frac{[2\mu(2j-1)^2 - 1 - 2\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]^{|n|}}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}\sin[(2j-1)\omega t]}{4\sum_{j=1}^{\infty}\frac{[\mu(2j-1)^2 - \sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}]}{\sqrt{\mu^2(2j-1)^4 - \mu(2j-1)^2}}}. \quad (26)$$

Convergence of all series is easily established by considerations literally similar to those presented above for solution (10). The only additional element for proof of consistency is the fact that no other bond besides w_0 is engaged in the impacts. According to Eq. (26), the deformation of the nth bond is expressed as

$$w_n(t) = Z(n+1,t) + Z(n-1,t) - 2Z(n,t). \quad (27)$$

The function $Z(n,t)$ has opposite signs for the neighboring particles; consequently, one obtains

$$|w_n(t)| = |Z(n+1,t) + Z(n-1,t) - 2Z(n,t)|$$
$$= |Z(n+1,t)| + |Z(n-1,t)| + 2|Z(n,t)|$$
$$\leqslant |Z(n+1,T/4)| + |Z(n-1,T/4)| + 2|Z(n,T/4)|. \quad (28)$$

However,

$$D = \max|w_0(t)| = |w_0(T/4)| = |Z(-1,T/4)| + |Z(1,T/4)| + 2|Z(0,T/4)|. \quad (29)$$

By virtue of Eqs. (13) and (26), quite obviously, for any $n \neq 0$ and $\mu > 1$ the sum of terms on the right-hand side of Eq. (29) is strictly larger than the last sum in Eq. (28). Therefore,

$$|w_n| < D, \quad n \neq 0, \quad \mu > 1. \quad (30)$$

Inequality (30) proves the consistency of solution (26) for the DB in the FPU-type model. Interestingly, the consistency of this solution follows from the consistency of solution (10) for the DB in the KG-type chain. Plots for maximum displacements $u_n(T/4)$ for two different values of μ according to solution (26) are presented in Figs. 3(a) and 3(b).

III. DISCUSSION

The solutions presented above can be significant as the benchmarks suitable for testing the approximations in the theory of the DB. Besides, the impact interaction is the high-energy limit for common models of the nonlinear lattices, such as the Toda lattice [24] or systems with Lennard-Jones

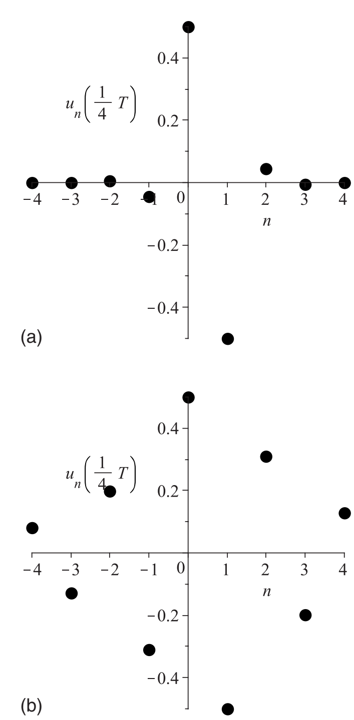

FIG. 3. Profile of the discrete breather (model of FPU type). Maximum amplitudes of the particles are plotted: (a) μ=3, (b) μ=1.05.

or Morse potentials. The role of the hard-point potentials as limit cases for more realistic potentials was outlined in [25]. Papers [26,27] discuss the shape and stability of the DBs in FPU-type lattices with strongly nonlinear nearest-neighbor interaction allowing the colliding-particles limit. The discrete breathers in the systems of this type in high-energy limits will be similar to the DBs derived in this paper.

The stability of solution (10) was verified by means of direct numeric simulations with parameters used for generation of Figs. 1(a) and 1(b). No detectable instability was revealed within more than 10 000 periods of oscillations in both cases. Such a simulation does not prove the stability rigorously. In order to analyze the stability in a rigorous manner, one should check the spectral properties of the linear dynamics around the DB. Such a problem seems to be rather complicated, due to both the singular nature of the problem and the infinite number of harmonics involved in the exact solution. Such a treatment is beyond the scope of the current work. From the numeric simulation, at least one can suggest that solution (10) is stable, as is the case for the DBs in similar systems [2,3,27].

To conclude, it is possible to find exact analytic solutions for the discrete breathers in both the nonintegrable chains of Klein-Gordon and Fermi-Pasta-Ulam types with vibroimpact potentials. These solutions are possible since the vibroimpact interaction can be rigorously reduced to the action of periodic external force on the linear lattice. Thus, these solutions can be easily generalized also for higher dimensions of the lattices, provided that the linear lattice is combined with appropriate impact interaction. Moreover, the method described above can allow for constructing more complicated solutions, such as coupled DBs or DBs with internal oscillating modes.

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[1] A. A. Ovchinnikov, Zh. Eksp. Teor. Fiz. **57**, 263 (1969).
[2] S. Flach and C. R. Willis, Phys. Rep. **295**, 182 (1998).
[3] S. Flach and A. Gorbach (unpublished).
[4] S. Aubry, Physica D **103**, 201 (1997).
[5] S. Aubry, Physica D **216**, 1 (2006).
[6] D. K. Campbell and M. Peyrard, in *CHAOS—Soviet American Perspectives on Nonlinear Science*, edited by D. K. Campbell (American Institute of Physics, New York, 1990).
[7] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[8] S. Takeno and A. J. Sievers, Solid State Commun. **67**, 1023 (1988).
[9] M. J. Ablowitz and J. F. Ladik, J. Math. Phys. **17**, 1011 (1976).
[10] A. A. Ovchinnikov and S. Flach, Phys. Rev. Lett. **83**, 248 (1999).
[11] Ya. G. Sinai, Russ. Math. Surveys **25**, 137 (1970).
[12] A. Rapoport, V. Rom-Kedar, and D. Turaev, Commun. Math. Phys. **272**, 567 (2007).
[13] B. V. Chirikov, Phys. Rep. **52**, 263 (1979).
[14] A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer, New York, 1992).
[15] D. Alonso, R. Artuso, G. Casati, and I. Guarneri, Phys. Rev. Lett. **82**, 1859 (1999).
[16] S. Denisov, J. Klafter, and M. Urbakh, Phys. Rev. Lett. **91**, 194301 (2003).
[17] O. V. Gendelman and A. V. Savin, Phys. Rev. Lett. **92**, 074301 (2004).
[18] V. I. Babitsky, *Theory of Vibro-Impact Systems: Approximate Methods*, Nauka, Moscow 1978 [Revised English translation, Springer-Verlag, Berlin, 1998].
[19] V. N. Pilipchuk, Int. J. Non-Linear Mech. **36**, 999 (2001).
[20] G. Casati, J. Ford, F. Vivaldi, and W. M. Visscher, Phys. Rev. Lett. **52**, 1861 (1984).
[21] L. I Manevitch, M. A. F. Azeez, and A. F. Vakakis, in *Dynamics of Vibro-impact Systems*, edited by V. I. Babitsky (Springer, Berlin, 1998); V. N. Pilipchuk, Nonlinear Dyn. **18**, 203 (1999).
[22] R. S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[23] L. I. Manevitch, C.-H. Lamarque, and E. Gordon, J. Appl. Mech. **74**, 1078 (2007).
[24] M. Toda, *Theory of Nonlinear Lattices* (Springer, Berlin, 1989).
[25] A. V. Savin, G. P. Tsironis, and A. V. Zolotaryuk, Phys. Rev. Lett. **88**, 154301 (2002).
[26] J. B. Page, Phys. Rev. B **41**, 7835 (1990).
[27] K. W. Sandusky, J. B. Page, and K. E. Schmidt, Phys. Rev. B **46**, 6161 (1992).