ASPECTS OF DISCRETE BREATHERS AND NEW DIRECTIONS

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Abstract
We describe results concerning the existence proofs of Discrete Breathers (DBs) in the two classes of dynamical systems with optical linear phonons and with acoustic linear phonons. A standard approach is by continuation of DBs from an anticontinuous limit. A new approach, which is purely variational, is presented. We also review some numerical results on intraband DBs in random nonlinear systems. Some non-conventional physical applications of DBs are suggested. One of them is understanding slow relaxation properties of glassy materials. Another one concerns energy focusing and transport in biomolecules by targeted energy transfer of DBs. A similar theory could be used for describing targeted charge transfer of nonlinear electrons (polarons) and, more generally, for targeted transfer of several excitations (e.g. Davydov soliton).

Keywords: discrete breathers, nonlinearity, discreteness, targeted transfer

1. INTRODUCTION

Discrete Breathers (DBs), also called Intrinsic Localized Modes, are spatially localized time-periodic solutions of discrete classical nonlinear Hamiltonian systems\(^1\). This self-localization is the consequence of model nonlinearity and discreteness independent of possible disorder. DBs are nonlinear modes which are rather universal and can be found in many finite or infinite systems of arbitrary dimension, which could be spatially

\(^1\)We do not consider in this paper DBs in dissipative systems which behave very differently and, in particular, can be dynamical attractors.
periodic, random, or else, and highly complex. Their detailed properties may be quite diverse and model dependent but up to now their investigation was mostly restricted to simple toy models. DBs, which are expected to exist in complex molecules or materials, could be studied through *ab initio* calculations.

Actually, their discovery has been predated by many early empirical works during the whole last century. For example, the concept of local modes was already introduced in chemistry for describing localized nonlinear vibrations in molecules long ago [1], was then forgotten and rediscovered [2, 3]. Polaron are also nonlinear objects belonging to the family of DBs introduced long ago by Landau [4]. In that case, the coupling of a quantum electron with a deformable medium may induce electronic self-localization by generating nonlinearities in the effective Schrödinger equation.

From the mathematical point of view, breathers were also found in some integrable models (Sine-Gordon) [5]. However, the breather solutions in these particular non-discrete models have the severe flaw to be non-generic because they disappear (as exact solutions) under most weak model perturbations. More recently, the discrete solitons of self-trapping equations, including Discrete Nonlinear Schrödinger Equations (DNLS), were intensively studied [3]. They could be viewed under many respects (but not all) as good prototypes of DBs. However, they have the peculiarity to be strictly monochromatic with only one frequency and no harmonics.

The first claim for the generic existence of DBs in nonlinear crystals was given by Sievers and Takeno (1988) [6]. However, it was still believed by many physicists that these solutions were only approximate and it was only in 1994 that their existence was rigorously established in infinite classical systems of coupled nonlinear oscillators [7].

The key mathematical property which makes DBs highly interesting in physics is that they are universal and correspond to *Exact, Robust and Linearly stable* solutions of classical nonlinear systems independent of their complexity. Classical DBs come as one parameter family parameterized by their frequency. Because of their universality, their analytic form can be rarely explicited, but they can be easily calculated numerically at any required accuracy in any given model where they exist [8]. Moreover, they are robust solutions, which means that they are not specific to Hamiltonians with a particular form. They persist as exact solutions of continuous families of models involving arbitrary potentials. They are linearly stable which means that any small perturbation of their initial conditions does not grow in time when treated linearly. This property does not imply the strict stability over very long
time but it guarantees that any small initial perturbation will grow much slower than exponentially in time. The linear stability property implies that when DBs are created in a nonlinear system on top of a quasi-linear thermalized background, they can persist over very long times that diverge when the temperature of the background becomes low.

In this short proceedings paper, we shall focus only on some aspects of DBs. We first recall the existence proof of DBs by continuation from an anticontinuous limit and then present some details concerning new existence criteria for hard DBs obtained by variational methods. We also discuss the existence of intraband DBs in systems that are both nonlinear and random with localized linear modes. We also briefly discuss the spontaneous formation of DBs in some out of equilibrium situations and also some exciting properties of DBs which may be targeted selectively from donor sites to acceptor sites in appropriate conditions.

2. EXISTENCE PROOFS FOR DISCRETE BREATHERS

The proof of existence of DBs essentially requires two ingredients:

- First, the system is truly nonlinear, i.e., the frequency of a mode depends on its amplitude (or, equivalently, its action).
- Second, the system is discrete so that the linear phonon spectrum exhibits gaps and does not extend up to infinite frequencies.

With these conditions, local modes may be found with frequency and its harmonics outside the linear phonon spectrum (see Fig.1). Then, it can be understood intuitively that since this local mode cannot emit any radiation by linear phonons (at least to leading order), the local mode energy remains trapped. This local mode may persist over very long time as a quasi-steady solution. Actually, we prove a stronger result under these assumptions, i.e., the existence of exact solutions with infinite lifetime.

These arguments make clear why the exact breather solutions in the Sine-Gordon model are non-generic. There are always breather harmonics in the linear phonon spectrum which extends up to infinity and the absence of linear radiation can be viewed as a highly exceptional phenomenon. Although DNLS equation is discrete, it is also particular, since for ensuring the existence of an exact solution it suffices that the fundamental frequency of the DBs (there are no harmonics) does not belong to the linear phonon spectrum.

The same arguments also suggest that the existence of quasiperiodic DBs in Hamiltonian systems with extended linear phonons, is also non-
Figure 1. (Scheme) When the fundamental frequency of a DB and all its harmonics
lie in the gaps of the linear phonon spectrum, no radiation is possible and the DB
solution persists with an infinite lifetime (at zero temperature).

generic. The reason is that the time Fourier spectrum of such a solution
is dense on the real axis and necessarily overlaps with the linear phonon
bands. As a result, it should radiate energy by phonon emission till the
solution either becomes time-periodic or vanishes.

Our initial method [7] for proving the existence of DBs works close
enough to a limit called anticontinuous, where the system decouples into
an array of uncoupled anharmonic oscillators and where the existence
of local modes is trivial. Then, the implicit function theorem can be
used for proving that this exact solution persists when the anharmonic
oscillators are coupled.

There are several ways for determining an anticontinuous limit for a
given model. These models can be classified in two classes. The first
class involves only optical modes with a phonon gap. The second class,
which is more realistic for real materials, involves acoustic phonons.

Methods using an anticontinuous limit. Let us consider as an
example of the first class, a Klein-Gordon chain with Hamiltonian

$$H_{KG} = \sum_i \frac{1}{2} u_i^2 + V(u_i) + \frac{C}{2} (u_{i+1} - u_i)^2$$  \hspace{1cm} (1)$$

where the atoms $i$ with scalar coordinate $u_i$ and unit mass are submitted
to an on-site potential $V(u_i)$ with zero minimum at $u_i = 0$ and are
elastically coupled to their nearest neighbors with coupling constant $C$. 
To fix the ideas, this local potential expands for small $u_i$ as

$$V(u_i) = \frac{1}{2}u_i^2 + \ldots$$

(2)

Then, the linear phonon frequency at wave vector $q$ is

$$\omega^2(q) = \sqrt{1 + 4C \sin^2 \frac{q}{2}}$$

(3)

which yields that the phonon spectrum is the interval $[1, \sqrt{1 + 4C}]$ and exhibits a gap $[0, 1]$.

An anticontinuous limit is obtained for this model at $C = 0$, when the anharmonic oscillators are uncoupled. Then, the motion of each oscillator is periodic and its frequency $\omega(I)$ depends on its amplitude or equivalently on its action $I$ (which is the area of the closed loop in the phase space $(u, \dot{u})$). Thus, we generally have $d\omega(I)/dI \neq 0$.

There are trivial DB solutions at the anticontinuous limit corresponding, for example, to a single oscillator oscillating at frequency $\omega_b$ while the other oscillators are immobile. If $n\omega_b \neq 1$ for any integer $n$, i.e., the breather frequency and its harmonics are not equal to the degenerate phonon frequency $\omega(q)$ at $C = 0$, the implicit function theorem can be used for proving that this solution persists up to some non-zero coupling $C$ as a DB solution at frequency $\omega_b$ [7].

More generally, even in complex models with an anticontinuous limit, the existence of DBs can be easily proven not too far from this limit [9, 10, 11].

However, models of the second class with acoustic phonons create problems because the phonon spectrum contains the frequency 0. Then, $n\omega_b$ always belongs to this phonon spectrum for $n = 0$. However, it was shown [12] that in molecular crystal models with harmonic acoustic phonons and non-vanishing sound velocity, the resonant coupling between the DB harmonics at $n = 0$ and the acoustic phonons becomes harmless and that the DB persists in the coupled system.

If one denotes as $y_i$, the coordinates describing molecule $i \in \mathbb{Z}^d$ on a $d$ dimensional lattice in its center of mass, $H_O(y_i)$ its Hamiltonian, and $x_i$, the coordinates of its center of mass, the Hamiltonian of such systems is assumed to have the form

$$H_{Mol} = \sum_i H_O(y_i) + k' \sum_{<i,j>} W(y_i, y_j)$$

$$+ \frac{1}{2} \dot{X}^t \cdot N \cdot X + \frac{1}{2} \dot{\mathbf{X}}^t \cdot M \cdot \dot{\mathbf{X}} + k \mathbf{Y}^t \cdot P \cdot \mathbf{X}$$

(4)

where $< i, j >$ denotes nearest neighbor molecules. In this expression, $X = \{x_i\}$ represents the set of variables called acoustic and $Y = \{y_i\}$
represents the set of internal variables of the molecules called optical. $k'W(y_i,y_j)$ represents a small direct nonlinear coupling between the optical variables of nearest neighbor molecules. The elastic energy of the crystal is assumed to be quadratic and characterized by the translationally invariant matrix $N$. $M$ is a diagonal matrix with the molecule mass $M$ as constant diagonal. There is also an elastic coupling energy with matrix $kP$ between the acoustic variables $X$ and the optical variables $Y$ obeying to translation invariance as well.

One gets an anticontinuous limit when coefficients $k$ and $k'$ are zero, i.e., the molecules are uncoupled. Then, the dynamics of acoustic variables uncoupled from the optical variables exhibit a standard gapless phonon spectrum with sound velocities generally depending on the direction in the crystal.

Then, it is proven [12] that if the uncoupled molecules exhibit a nonlinear mode (i.e., a time-periodic solution) with frequency and harmonics $n\omega_b$ that do not belong to the acoustic phonon spectrum for any non-zero integer $n$, and are not equal to any of the linear (i.e., normal) modes of the isolated molecule (for any $n$), then the coupled system with $(k,k') \neq 0$ not too large does exhibit DB solutions. Only generic assumptions are necessary for this result (non vanishing-sound velocities and dependence of the frequency of the nonlinear mode of the molecule on the action).

These DBs are obtained by continuation with respect to $k$ and $k'$ of the time-periodic solution at $(k,k') = 0$ where a single molecule oscillates (see Fig.2). Their frequencies may belong to the gap(s) between the linear acoustic modes and the linear optical modes or may be above the whole phonon spectrum. However, it is important to note that while the dynamical part of the DB decreases exponentially, the DB behaves like a static impurity, i.e., there is generally a static component which decays with a power law (two and more dimensions).

Another technique for proving the existence of DBs in diatomic FPU models was used in [13]. The Hamiltonian of such models has the form

$$H_{FPU} = \sum_i \frac{1}{2} m_i \ddot{u}_i^2 + W(u_{i+1} - u_i)$$

(5)

where $m_i = m$ for $i$ even and $m_i = M$ for $i$ odd. $W(x)$ is an anharmonic convex potential. An anticontinuous limit for this model is obtained for a zero mass ratio $m/M$. The dynamical equation of this system is

$$m_i \ddot{u}_i + W'(u_i - u_{i-1}) - W'(u_{i+1} - u_i) = 0$$

(6)

When the mass of the heavy odd atoms $M$ goes to infinity, a solution of these equations is obtained for $u_{2i+1}$ time-independent ($\ddot{u}_{2i+1} = 0$).
The nonlinear mode of an isolated anharmonic molecule may persist in the crystal as a DB when there are no resonances between its frequency (and harmonics) and the linear phonon modes of the whole system.

The dynamical equations for the light even atoms decouple

\[ m\ddot{u}_{2i} + W'(u_{2i} - u_{2i-1}) - W'(u_{2i+1} - u_{2i}) = 0 \]

so that the motion of the even atoms \( 2i \) are those of uncoupled anharmonic oscillators with fixed potential \( W(u_{2i} - u_{2i-1}) + W(u_{2i+1} - u_{2i}) \).

The simplest DB at this limit corresponds to a single even atom oscillating in the chain while the heavy atoms are relaxed at static equilibrium. Then, under standard non-resonance conditions (and omitting technical details), the implicit function theorem also states in this case, that this time-periodic solution persists when \( M \) is not infinite but only large enough. However, this approach cannot prove the existence of a DB solution when the mass ratio becomes unity (\( M = m \)).

Variational methods. A flaw of the methods proceeding by continuation of DBs from an anticontinuous limit is that it is generally difficult to estimate explicitly the domain of parameters where DBs persist (although this can be easily tested numerically). This is the reason why we started a new approach based on variational methods [14] which yields criteria ensuring the existence of DBs for a given model at given parameters. This variational approach is inspired from the existence criteria for polarons (which can also be used for DNLS models). In this simpler case, it suffices to exhibit a wavefunction with variational energy smaller than the bottom of the electronic band.

Up to now, we found such a criterion for some classes of models proving only the existence of hard DBs (i.e., with frequency above the linear phonon spectrum). As an application, this criterion can be used for
the above FPU diatomic chain when the potential \( W(x) \) is hard (i.e., when \( W(x) \) diverges faster than \( x^2 \) for large \( x \)). Then, there are DBs at large enough frequencies. Moreover, in special cases, like the 1D \( \beta \)-FPU model where \( W(x) = x^2/4 + x^4/4 \), it can be proven with our criterion that there are DBs with frequencies infinitely close to the acoustic phonon band edge. Note that this result is not valid for \( \beta \)-FPU models in two and more dimensions, where it is known that there is an energy threshold for DBs \([15]\). Our criterion can be used (or easily extended) for complex Hamiltonians on periodic lattices with massive particles with hard DBs.

This criterion applies to translationally invariant Hamiltonians describing atoms on a periodic lattice, e.g. \( \mathbb{Z}^d \), submitted to a potential with local interactions which is convex at least in some vicinity of its ground-state \( u_i \equiv 0 \). In order to fix the ideas, we consider for example the form

\[
H = \sum_i \frac{1}{2} u_i^2 + V(u_i) + \sum_{<i,j>} W(u_j - u_i) \tag{8}
\]

where \( u_i \) are scalar variables describing the displacements of particles with mass unity (taken equal for simplicity) and where \( V(x) \) and \( W(x) \) are anharmonic convex functions. We can set \( V(x) \equiv 0 \) for obtaining a model of the second class with acoustic phonons. Despite the fact that we have to construct different proofs for the two cases, the final criterion for DB existence is the same. Then, Klein-Gordon chains and FPU models correspond to special cases of this model.

We define first for \( \mathbb{C}_2 \), \( 2\pi \) periodic loops \( \{u_i(\varphi)\} \) (i.e., twice differentiable with respect to \( \varphi \) with continuous derivatives), a quantity we call “pseudoaction”

\[
J(\{u_i(\varphi)\}) = \frac{1}{2\pi} \int_0^{2\pi} \sum_i \left| \frac{du_i}{d\varphi} (\varphi) \right|^2 d\varphi \tag{9}
\]

and the average energy

\[
E(\{u_i(\varphi)\}) = \frac{1}{2\pi} \int_0^{2\pi} \left( \sum_i V(u_i(\varphi)) + \sum_{<i,j>} W(u_j(\varphi) - u_i(\varphi)) \right) d\varphi \tag{10}
\]

It is straightforward to prove that the extrema of the average energy \( E(\{u_i(\varphi)\}) \) in the space of loops at fixed pseudoaction \( J(\{u_i(\varphi)\}) \) are invariant loops for the dynamics associated with Hamiltonian (8). More
precisely, if \( \{ u_i(\varphi) \} \) is such an extremum then for

\[
\omega_0^2 = \frac{\int_0^{2\pi} \sum_{i,j} \frac{d u_i}{d \varphi} \frac{\partial^2 V}{\partial u_i \partial u_j} \frac{d u_j}{d \varphi} d\varphi}{\int_0^{2\pi} \sum_i \left( \frac{d^2 u_i}{d \varphi^2} \right)^2 d\varphi}
\]  

(11)

\( \{ u_i(\omega b t) \} \) is a spatially localized time-periodic solution of the system, i.e. a DB solution. We prove the existence of extrema and thus of DBs by minimax methods when the following simple criterion is fulfilled:

**Existence Criterion for DBs:** Let us assume that for a given Hamiltonian, we can exhibit one loop \( \{ a_i(\varphi) \} \) with zero average, i.e., such that for any \( i \),

\[
\int_0^{2\pi} a_i(\varphi) d\varphi = 0
\]  

(12)

and such that we have the inequality

\[
E(\{ b_i + a_i(\varphi) \}) > \frac{1}{2} \Omega^2 J(\{ a_i(\varphi) \})
\]  

(13)

for any vector \( \{ b_i \} \) (independent of \( \varphi \)). Then, there exists an invariant loop \( \{ u_i(\varphi) \} \) (a DB solution) such that \( J(\{ u_i(\varphi) \}) \leq J(\{ a_i(\varphi) \}) \).

For given models, when potentials \( V(x) \) and \( W(x) \) are symmetric, it is often easy to test this criterion by choosing sine loops \( a_i(\varphi) = c_i \cos \varphi \) because the minimum of the convex function \( E(\{ b_i + c_i \cos \varphi \}) \) of \( \{ b_i \} \) is obtained for \( b_i \equiv 0 \). Then, it suffices to test the condition \( E(\{ a_i(\varphi) \}) > \frac{1}{2} \Omega^2 J(\{ a_i(\varphi) \}) \) by calculating explicitly the average energy (10) for this specific loop as a function of \( \{ c_i \} \). In models where hard DBs can be found numerically, it is generally easy to choose a DB shape \( \{ c_i \} \) which roughly approaches the shape of the real DB and to test if it fulfills the DB existence criteria. Choosing \( c_i = 0 \) except for \( c_0 \) is often sufficient when \( c_0 \) is large enough. One can also use the approximate solution obtained from Rotating Wave Approximation methods, for finding trying loops.

When, the potentials are not symmetric, a simple trick consists of replacing the initial potentials by symmetrized potentials \( V_S(x) = V_S(-x) \leq V(x) \) and \( W_S(x) = W_S(-x) \leq W(x) \) for all \( x \) defined by

\[
V_S''(x) = \min V''(x), V''(-x) \quad V_S'(0) = 0 \quad V_S(0) = 0
\]  

(14)

\[
W_S''(x) = \min W''(x), W''(-x) \quad W_S'(0) = 0 \quad W_S(0) = 0
\]  

(15)
Then, if criterion (13) is fulfilled for these new symmetric potentials, it is fulfilled for the initial ones

\[ E_S(\{u_i(\varphi)\}) = \frac{1}{2\pi} \int_0^{2\pi} \left( \sum_i V_S(u_i(\varphi)) + \sum_{<i,j>} W_S(u_j(\varphi) - u_i(\varphi)) \right) d\varphi \leq E(\{u_i(\varphi)\}) \] (16)

It comes out very generally that if potential \( V(x) \), or \( W(x) \), or both, grow faster than \( x^2 \), the DB existence is granted at large enough frequency above the phonon band. However, at the present stage, we only proved that the pseudoaction of the invariant loop is smaller than or equal to the pseudoaction of the initial trying solution. The strict equality is not true in general as confirmed by examples with models where the potentials are not “hardening” at large amplitude. However, we expect to prove the equality if the potentials are “hard enough” but this needs a correct definition within a general formalism.

The extension of this criterion is straightforward when the variables \( u_i \) are not scalar. Then, we can describe realistic crystal structures with many different atoms per unit cell and different masses. We plan to modify our minimax techniques for finding modified criteria proving the existence of soft DBs (i.e., with frequencies inside the linear phonon gaps).

It appears that the existence of DBs can be rigorously proven in an increasing number of classes of models independent of their complexity and thus the concept of DB is rather universal.

**Discrete breathers in random systems and Anderson modes.**

When the Hamiltonian system is random (for example an array of random anharmonic oscillators), there is no mathematical difference concerning the DB existence proof from the anticontinuous limit when the frequency of the DB and its harmonics do not belong to the linear phonon spectrum. These DBs are called extraband DBs.

When the linear modes are localized due to disorder (Anderson modes), it becomes an interesting question to understand the interplay between localization due to disorder and localization due to nonlinearity. It was demonstrated [16, 17] that disorder and nonlinearity in the same system play a *double game*. For some time-periodic solutions, they cooperate for maintaining mode localization thus generating intraband DBs. However, there are other time-periodic solutions which are spatially extended and which can transport energy. The reasons is that resonances between oscillators with different frequencies can be restored by the nonlinearities, since their effective frequencies can be tuned by their amplitude.
For understanding the subtlety of this effect and its complexity, it is necessary to involve time-periodic solutions which are not single DBs. These solutions can be easily found at the anticontinuous limit by choosing an arbitrary subset of the uncoupled nonlinear oscillators (finite or infinite) oscillating at the same frequency. It can be proven in the same way as for the single DBs [10] that when their frequency and harmonics do not belong to the linear phonon spectrum (for periodic systems as well as for random systems) these so-called multiDB solutions persist up to some non-vanishing coupling as exact solutions. Among them, there is an infinite number of linearly stable multiDB solutions [10].

We investigated in refs.[16, 17], on the base of a combination of numerical and analytical arguments how the frequency of these exact solutions could penetrate the phonon spectrum when it is discrete (for example when the model randomness is large enough). We obtained the following generic conclusions:

- Any extraband single DB or any spatially localized multiDB systematically disappears by bifurcating with another multiDB before its frequency penetrates or just when reaching the linear phonon band edge. This bifurcation is caused by the resonance between the DB frequency and the linear Anderson modes with frequencies close to the band edge.

- There are spatially extended time periodic solutions obtained by continuation of certain multiDBs while their frequency enters the phonon spectrum till a certain intraband frequency. At this point, the multiDBs also disappear by bifurcating with another multiDB. These multiDBs are characterized by the fact that the sites where the linear modes associated with the encountered linear resonances are located, are occupied by DBs (with appropriate phases). As a result, the resonance with the linear mode becomes ineffective.

- Some of these multiDBs can be continued to the linear limit at zero amplitude but remain extended modes. Conversely, the strict continuation of localized linear Anderson modes at nonzero amplitude is possible but it yields immediately extended (but sparse) multiDBs as soon as the amplitude is non-zero.

- However, each localized linear Anderson mode could be continued but in an approximate sense only as a spatially localized intraband DB but there is a (generally) small discontinuity, each time its frequency crosses a linear mode frequency. Obviously, the resonance with the linear mode would transfer the DB energy to this mode thus defocusing its energy and destroying the DB. Since this set
of linear frequencies is dense inside the phonon band, there are infinitely many gaps in the set of frequencies where this intraband DB could persist. However, it has been proven in some models that this set of frequencies is non-void. It is a fat Cantor set with non-zero Lebesgue measure. Moreover, in the limit of small DB amplitudes where nonlinearities becomes weak, the gap widths of this Cantor set tend to vanish so that this Cantor set tends to be full.

3. PERSPECTIVES ON DISCRETE BREATHERS APPLICATIONS

**Manifestation of DBs in out of equilibrium states.** Because DB solutions are robust and linearly stable, they may show up spontaneously in molecular dynamics simulations in nonlinear models, where they exist, especially in situations where they are out of equilibrium.

Such situations are obtained for example when a relatively big amount of energy is deposited locally (for example by a photon absorption). Tight-binding molecular dynamics on hydrocarbons clearly show that when vibrational energy is deposited locally on a proton, it remains localized over very long times. The frequencies of the anharmonic, localized and time-periodic vibrations do not correspond to normal modes, which strongly suggests that they are DBs [18]. These and similar phenomena are invoked for explaining observed anomalous infrared radiation of interstellar dust [18, 19]. DNLS systems with initial configurations very far from equilibrium do not thermalize and spontaneously exhibit DBs [20]. Moreover, norm conservation makes that for some initial conditions, DNLS systems cannot thermalize [21] and induces the formation of DBs.

Sharp thermal shocks [22, 23] also exhibit clearly the formation of DBs. The example shown in Fig.3 was described in ref.[23]. It is obtained for a 2D array of coupled quartic oscillators which can sustain DBs. Initially, the system is at thermal equilibrium at a high enough temperature in order for the energy involved in the anharmonic terms to be relatively important. At time zero, the boundaries of the system are suddenly cooled down to zero K (by damping the motion of the atoms close to the boundary). If the system were harmonic, we would expect that the total energy of the system would decay exponentially as \( E(t) \approx E(0) \exp(-t/\tau) \) with some characteristic time \( \tau \) according to the Fourier law. Actually, the observed energy decay is much slower and can be well fitted by a stretched exponential \( E(t) \approx E(0) \exp(-\alpha t^\beta) \), where the coefficients \( \alpha \) and \( \beta \) depend on the initial temperature. If
one observes the evolution of the spatial pattern of the energy density in the system, one finds that after a relatively short time, it consists of narrow peaks which fit remarkably well with exact DB solutions. It is then clear why the energy remains trapped in the system. In the DB regime, the energy transport towards the absorbing boundaries essentially originates from the overlap of the DBs tails which may generate traveling phonons from their frequency interference. Since this interaction becomes weaker and weaker as the DBs density decreases and their relative distance increases, the rate of the energy relaxation decreases as a function of time.

This long lifetime of intraband DBs should be also useful for understanding many anomalous energy relaxation phenomena in disordered materials (glasses, polymers, biopolymers). Thermal shocks as shown above have been also performed in nonlinear random systems with linear Anderson modes thus implying the existence of intraband DBs [24]. Again, a slow relaxation of the energy due to energy trapping by intraband DBs can be observed similar to Fig.3. However, in contrast with the periodic crystal, the anomalous relaxation not only persists but it dramatically slows down when the initial temperature gets small, i.e.,
the system becomes close to linear. This effect can be expected because unlike the periodic crystal, the linear Anderson modes cannot propagate at all and energy propagation is essentially due to nonlinearities (the existence of extended multiDBs demonstrate this possibility). More generally, any small thermal shock between two different non-zero but small temperatures reveals energy relaxation which becomes extremely slow when the temperature drops and no thermalization can be reached within computable times. This numerical experiment suggests that there is no need to invoke static metastable configurations (usually modeled by two-level states) for interpreting the slow relaxation properties of real glasses since random models without metastable states but with only some weak nonlinearity, are sufficient for exhibiting a glassy behavior at low temperature.

**Targeted Energy Transfer.** Another very interesting property of DBs is that in some cases they could transport energy between donor and acceptor sites in a highly selective way. The extended dimer model described in [25] can be used for describing the transfer of energy as DBs for lattice vibrations, electrons (polarons), excitons or many other kinds of excitations. It is thus highly relevant for chemical reactions and particularly bioenergetics which involves such transfers between different atoms, molecules, or macromolecules.

Let us briefly sketch the mechanism of Targeted Energy Transfer (TET) between two anharmonic oscillators.

Resonance is the basic principle for energy transport in harmonic systems. The simplest example in textbooks is obtained for two weakly coupled identical harmonic oscillators. Then, any amount of energy deposited on one of the two oscillators slowly tunnels back and forth between these two oscillators with a frequency proportional to the coupling.

When the oscillators are anharmonic, their frequency depends on its amplitude. Therefore when starting the energy transfer the linear frequency of the second (acceptor) oscillator should be approximately equal to the frequency of the donor oscillator oscillating at non-zero amplitude. But while the energy transfer begins the frequencies of the oscillators change because of the change of their oscillation amplitudes and they generally become unequal. Thus, the energy transfer stops much before it becomes complete. However, there are fine tuned cases where the resonance persists during the energy transfer which then can become complete. We found an analytic model for describing precisely this situation. We call this exceptional but very important phenomenon Targeted Energy Transfer because it is highly selective. In large systems
consisting of many coupled anharmonic oscillators, it may occur only for a given amount of energy and for a selected pair of anharmonic oscillators called Donor and Acceptor. We can also determine the critical coupling beyond which this energy transfer occurs.

The Donor and Acceptor oscillators are described with action-angle variables $I_D, \theta_D$ and $I_A, \theta_A$ with Hamiltonian $H_D(I_D)$ and $H_A(I_A)$. Then, the weak coupling is a function of $C(I_D, \theta_D, I_A, \theta_A)$ and the total Hamiltonian is

$$H_{Dim}(I_D, \theta_D, I_A, \theta_A) = H_D(I_D) + H_A(I_A) + C(I_D, \theta_D, I_A, \theta_A) \quad (17)$$

Since this coupling is assumed to be weak, we are close to an adiabatic limit where the total action is $I_T = 2I_0 = I_D + I_A$ is conserved and the half difference $I = (I_D - I_A)/2$ varies slowly. The conjugate variables to $I_0$ and $I$ are $\theta_0 = \theta_D + \theta_A$ and $\theta = \theta_D - \theta_A$, respectively. We are allowed to average Hamiltonian (17) over $\theta_0$ which is a fast variable so that we obtain an integrable Hamiltonian with the form

$$H_T(I_0, I, \theta) = H_0(I_0, I) + V(I_0, I, \theta) \quad (18)$$

where $I_0$ (which is time-constant) becomes a parameter. $H_0$ is defined as $H_0(I_0, I) = H_D(I_0 + I) + H_A(I_0 - I) + V_0(I_0, I)$ so that the average over $\theta$ of $V(I_0, I, \theta)$ is zero.

For having a solution where $I(t)$ varies from $I_0$ to $-I_0$, thus corresponding to a complete energy transfer between the two anharmonic oscillators, the energy must be conserved, which implies that unlike the harmonic case, it may occur only at specific energies $E_T$ when $I_0$ fulfills

$$H_0(I_0, I_0) = H_0(I_0, -I_0) = E_T$$

With the reasonable assumption that the effective coupling $V(I_0, I, \theta)$ is a sine-like function of $\theta$ (that is it has only one maximum and one minimum per period when $|I| \leq I_0$), we prove moreover that the inequality

$$\min \theta V(I_0, I, \theta) < \epsilon_T(I) = H_0(I_0, I) - H_0(I_0, I_0) < \max \theta V(I_0, I, \theta) \quad (19)$$

is a necessary and sufficient condition for the existence of TET solution. Function $\epsilon_T(I)$, defined for $|I| \leq I_0$ and such that $\epsilon_T(I_0) = \epsilon_T(-I_0) = 0$, is called detuning function. It may be positive, negative or change its sign in the interval $|I| < I_0$.

Targeted Energy Transfer can be obtained at low coupling for a specific energy, only if the variation of the detuning function is small, which requires appropriately chosen Donor and Acceptor oscillators (particularly, one should be soft while the other is hard or vice versa). A 3D plot
of the transfer rate between two anharmonic oscillators versus energy $E_T$ and action $I_T$ is shown in Fig.4 for a DNLS dimer model where the detuning function is strictly zero [25]. It demonstrates the high selectivity of the transfer.

DBs are continuous families of classical solutions which are parameterized by their frequency, or better, their action $I$ with a total energy $H(I)$. Each DB family behaves as the periodic solutions of an anharmonic oscillator with Hamiltonian $H(I)$ in action angle representation ($\theta$ denotes the variable conjugate to $I$). The DB (and multiDB) families are different if the systems are non-periodic. Then, in practice, conditions (19) for TET can be tested numerically for two nonlinear systems (finite or infinite) initially uncoupled by calculating the energy function $H(I)$ for each pair of DBs families on the acceptors. These systems physically represent two molecules or macromolecules Donor and Acceptor. Then, one can detect pairs of DBs with small detuning functions. Numerical examples presented in ref.[26] confirm that for an appropriate amount of energy deposited as a specific DB on the donor molecule, this energy can be completely transferred as another specific DB on the acceptor molecule while the intermolecular coupling is only 2% of the intramolecular coupling. Because of the high energy selectivity, a small energy dissipation during the transfer could be sufficient for making TET irreversible. Cascades of TET along specific chains of DBs linked in a specific order could be constructed as well as funneling of DBs toward specific centers. We can also imagine energy stacking of DBs, etc.

The same theory can be used for describing the adiabatic transfer of a quantum electron (or other kind of excitations such as a Davydov exciton) between two molecules. In this case $I_D$ (resp. $I_A$) represents
the fraction of the electron on the Donor (resp. Acceptor) molecule while $H_D(I_D)$ (resp. $H_A(I_A)$) is the energy of the Donor molecule for this fractional charge (which can be defined within density functional theory). Thus, TET theory could be used for understanding chemical reactions and catalysis, especially for enzymes in biochemistry.

The new directions of applications we briefly suggested in this paper, confirm the potential richness of the theory of Discrete Breathers and its extensions. It could become a powerful paradigm for investigating a wide variety of physical phenomena in physics, chemistry and biophysics.

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