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Review

Discrete Breathers: Localization and transfer of energy in discrete Hamiltonian nonlinear systems

S. Aubry*

Laboratoire Léon Brillouin (CEA-CNRS), CEA Saclay, 91191 Gif-sur-Yvette Cedex, France

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Abstract

We present a partial review of results concerning the theory of Discrete Breathers in nonlinear hamiltonian and discrete systems. These special time-periodic solutions gained much interest during the last decade because they may be involved in numerous and various phenomena in physics and biophysics where they could produce nontrivial effects of energy focusing and transfer. We first review the principles which govern their existence and which are used in the existence proofs available up to now. Next we discuss their linear stability and the interaction of Discrete Breathers with small amplitude waves, showing also how they could grow or decay. We also briefly discuss the existence of intraband DBs in systems with a linear discrete spectrum which are not spatially periodic (random or otherwise) and where linear waves cannot propagate. We also show that nonlinearity may restore the existence of solutions that propagate energy. We review some results concerning energy transportation by DBs and especially the main features associated with their mobility. We briefly discuss new perspectives opened up by the theory for applications that, in particular, look especially interesting for biophysics.

Keywords: Discrete breathers; Polarons; Nonlinear dynamics; Mobility; Energy focusing; Energy transport

1. Introduction

First, I would like to acknowledge the organizers of this symposium dedicated to my 60th birthday, for the honor they gave me. The purpose of this paper is a partial review of the works in which I participated concerning the theory of Discrete Breathers (with the opportunity to mention a few extra unpublished results). I would also like to discuss future prospects concerning applications to some puzzling problems of physics and, especially, biophysics.

According to standard phenomenological theories that can be found in textbooks, it is usually believed that, when some energy is injected into a physical system, it will relax spontaneously at thermal equilibrium according to the standard diffusion laws of heat. The most common assumption underlying standard theories that describe the dynamics of systems close to thermodynamical equilibrium is that the unknown consequences of the complexity and the nonlinearities of these systems on the energy redistribution can be modelled at the microscopic level by a damping and an associated random (Langevin) force. This concept of a Langevin phonon bath has surely been the most convenient way to get rid of the complex nonlinear dynamics that may occur during energy thermalization and, moreover, it has produced a great number of successful theories sufficient for understanding many phenomena.

For example, the modern theory of chemical reactions based on Kramers theory [1,2] describes ordinary chemical reactions by a Brownian particle (representing the configuration of the system in a large space) climbing an energy barrier between two energy wells (where the first well represents the state of the reactant molecules and the second well those of the product molecules). The thermal fluctuations are modelled by a friction and a Langevin random force acting on this particle.

Other theories of chemical reactions for unimolecular systems [3,4] (involving only a few degrees of freedom) also assume fast Intramolecular Vibrational Redistribution (IVR) at the time scale of the chemical reaction (RRKM theory) [5].

* Tel.: +33 169086128; fax: +33 169088261.
E-mail address: saubry@dsm-mail.saclay.cea.fr.

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A typical trajectory is supposed to explore all the energetically accessible reactant phase space.[1]

Actually, the standard theories for non-equilibrium phenomena, which are still prevalent today, assume that the dynamics of nonlinear systems is strongly chaotic in phase space, which thus can be rapidly explored from any initial conditions. This assumption seems to be supported by the fact that KAM theories that predicts the existence of quasiperiodic and non-chaotic trajectories are restricted to finite systems and do not hold for infinite systems, where chaos is believed to be prevalent. Nevertheless it seems that, even in infinite systems, there are many weakly chaotic trajectories close to special solutions such as time-periodic solutions (Discrete Breathers) which may trap the system for very long time and could retard full thermalization over very long time.

Numerical investigations of discrete (non-integrable) nonlinear systems now demonstrate that there may exist many such solutions cluttering up the phase space and, moreover, that this property is not restricted to exceptional models but is rather universal. These results could question the validity of the standard theories describing out-of-thermal-equilibrium phenomena. The first historical example goes back to the famous numerical experiment of Fermi et al. [9] performed on a simple one-dimensional chain of identical atoms coupled with anharmonic springs. They found the absence of thermalization of an initial long wavelength perturbation over very long time. It has been shown later that the FPU model that they investigated can be very well approximated by an integrable model with solitons (KdV), which explains its slow thermalization.

Actually, slow thermalization is a more general phenomena. It may also occur because of energy self-trapping phenomena. It is well known from those familiar with molecular dynamic calculations that generally nonlinear systems do not thermalize spontaneously by themselves within a reasonably short computer time if the initial state is too far from thermodynamical equilibrium. It is usual to accelerate the thermalization process for practical reasons with various algorithms (coupling with a Langevin bath, Nosé method etc...). Actually, these methods are artificial and generally do not correspond to any real physical dynamics of the system.

It is thus challenging to understand these non-equilibrium phenomena through the most recent advances of nonlinear physics. Many recent works initiated by the pioneering paper of Sievers and Takeno [10] confirmed that energy localization is a ubiquitous phenomenon in discrete nonlinear systems [11]. Energy Localization occurs because of the spontaneous formation of Discrete Breathers (DBs) [12], called originally [10] *Intrinsic Localized Modes* (ILM). These DBs are exact spatially localized time-periodic solutions of discrete nonlinear Hamiltonian systems [13,14] which are often linearly stable. This existence of DBs in a model is not related to some specific but exceptional properties but occurs generally because of the interplay of nonlinearity and discreteness. Discrete DB may exist in models at any dimension, although in two and more dimensions (with short range interactions), an energy gap is required for their creation [15].

Thus, when a system possesses linearly stable DB solutions, they are able to maintain energy trapped over unexpectedly long times. It is worthwhile noting that the self-trapping of electrons (or, more generally, quantum excitations) in deformable media as polarons [16] is a closely related phenomenon (where nonlinearity is also essential) which has already been known for many decades. In particular, the Davydov theory of polarons [17], proposed for the understanding of energy focusing and transportation in α-helix proteins, has been studied intensively over the last two decades [18,19].

Direct observation of energy localization has now been obtained in a number of macroscopic systems that were intentionally built and well described by nonlinear and discrete dynamical equations [20–23]. There is indirect evidence at the microscopic scale in several very different microscopic systems [24–29] but DBs have not been observed directly.

Although the phenomenon of energy localization due to nonlinearity and discreteness is now well established from the theoretical point of view, the direct measurement of energy localization at the atomic scale in real systems is still beyond the frontier [30]. Nevertheless, we think that DB theory and related concepts have to play an important role in condensed matter physics.

The aim of this paper is to present a partial review of the theory of DBs. Section 2 describes the general principles of the proofs for the existence of DBs that have been available up to now. We also discuss their linear stability (Section 3) and present some numerical simulations (Section 4) where DBs show up spontaneously. Section 5 discusses the interaction of DBs with small amplitude waves and gives some insight into how DBs could grow or decay. Section 6 discusses the existence of DBs with frequencies inside a discrete linear phonon spectrum (Intraband Discrete Breathers or IDBs). Section 7 is devoted to energy transportation by DBs. We mostly discuss DB mobility and energy transportation by multi-DBs by phase torsion. Targeted Energy Transfer is only briefly mentionned because of the lack of time and should be reviewed in further publications. Finally, the conclusion (Section 8) briefly discusses the perspectives opened up by the theory of Discrete Breathers and related phenomena.

2. DBs existence proofs

We briefly describe the basic principles involved for obtaining rigorous results. The existence of DBs has been proven rigorously with several mathematical methods in a large variety of models with optical or acoustic phonons, with or without gaps, in one or any dimension and with or without randomness [31–36]. Usually, these models deal with interacting massive classical particles (atoms) obeying Hamiltonians with the form

$$\mathcal{H} = \sum_i \frac{p_i^2}{2} + \mathcal{V}(\{u_i\}) \tag{1}$$

[1] However, recent papers pointed out that the reaction dynamics may be *extremely nonstatistical* in some cases [6–8] which was empirically interpreted by the existence of IVR bottleneck.