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Interaction of discrete breathers with thermal fluctuations

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Discrete breathers (DB) are time-periodic and spatially localized lattice excitations, which can be linearly stable or unstable with respect to either localized or extended perturbations. We analyze the interaction of DBs with a thermalized background of small amplitude lattice excitations in a one-dimensional lattice of Morse oscillators with nearest neighbour interaction. We find that stable DBs are barely influenced by the thermal noise. Unstable DBs are starting to propagate through the lattice, without loosing their localization character. The instability can be both due to localized perturbations, as well as due to extended perturbations. We discuss these observations in terms of resonances of DBs with localized and delocalized perturbations, and relate them to the issue of DB impact on statistical properties of nonlinear lattices.

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1. Introduction

Discrete Breathers (DBs) or Intrinsic Localized Modes (ILMs) are time periodic and spatially localized excitations which generically exist in the presence of spatial discreteness and nonlinearity [1]. First results have been obtained more than 30 years ago by Ovchinnikov [2] and Kosevich and Kovalev [3]. DBs were numerically observed by Sievers and Takeno [4] in 1987. More than a decade of recent intense studies lead to existence proofs of DBs [5], computational methods of obtaining DBs in classical and quantum systems (for references see [6]), and to many other results on e.g. stability, dynamics, mobility of DBs (for references see [1]). DBs have been observed experimentally in various physical settings, e.g. in Josephson junction networks [7,8], in PtCl crystals [9], in quasi-one dimensional antiferromagnets [10], in micromechanical cantilever arrays [11], in optical waveguide networks [12,13], and in Bose–Einstein condensates on optical lattices [14]. Theoretical predictions of DB existence range from excitations in metamaterials [15] to oscillations in dusty plasma crystals [16].

Another important theoretical aspect of DBs concerns their impact on statistical properties of nonlinear lattices. They are known to spontaneously form in the transient process of relaxation of a nonequilibrium state towards equilibrium, and thereby to significantly slow down the whole process. Prominent examples are: i) the excitation of an extended plane wave, which undergoes modulational instability and fragments into DB-like hot spots and a cold background of delocalized waves [17,18], and ii) the radiation of a thermalized part of a lattice into a cold exterior, which leaves DB-like excitations inside the originally thermalized volume untouched for long times [18,19]. DB-like excitations are also spontaneously created and destroyed in lattices in thermal equilibrium [21]. A number of numerical studies were devoted to detect and analyze the statistical properties of these excitations [18,20–22].

In this work we aim at a controlled observation of the interaction of a single DB embedded in a thermalized lattice. We will study how the outcome depends on the linear stability of the DB under consideration. In Sec. 2 we describe the DB construction and stability, and the expected consequencies on the interaction of DBs with a thermal environment. In Sec. 3 we simulate a thermalized system adding a linear stable or unstable DB and study the interaction of the DB with the thermal fluctuations. In Sec. 4 we discuss the results and conclude.

2. DB construction and stability

We compute discrete breathers (DBs) using the well known method of the anticontinuous limit [23] in a lattice of $N = 120$ sites of nearest neighbor interaction and Morse on-site potential (see also [6]). The equation of motion for the site i reads

$$\ddot{x}_i = k(x_{i+1} + x_{i-1} - 2x_i) - (1 - e^{-x_i})\, e^{-x_i}, \qquad (1)$$

where k is the coupling between the nearest neighbors. For a frequency $\omega_b = 0.863$ and a coupling between the nearest neighbors $k = 0.1$, a linearly stable breather exists while for the same value of frequency but for a value of coupling $k = 0.16$ a linearly unstable breather is found. The stability is determined by calculating the eigenvalues and eigenvectors of the Floquet matrix, which characterizes the linearized phase space flow around a DB [6,23]. Note that the Floquet spectrum contains two continuous arcs, and a discrete part. The continuous arcs correspond to extended small amplitude waves with frequencies $1 \le |\omega_q| \le \sqrt{1+4k}$. For the DB to exist, we need to satisfy $m\omega_b \ne \omega_q$ for all integers m. While respecting that nonresonance condition, the overlapping of the two continuous arcs may take place, and will correspond to a resonant coupling of two plane waves, mediated by the DB: $\omega_{q_1} = \omega_{q_2} + m\omega_b$.

The results of the Floquet analysis are shown in Fig. 1,*a* where the eigenvalues of the Floquet matrix are depicted for both cases of couplings ($k = 0.1$ and $k = 0.16$). In the lower panel (Fig. 1,*b*) we plot the amplitude of the corresponding DBs as a function of the lattice site (at some initial time, at which all velocities $\dot{x}_i$ vanish).

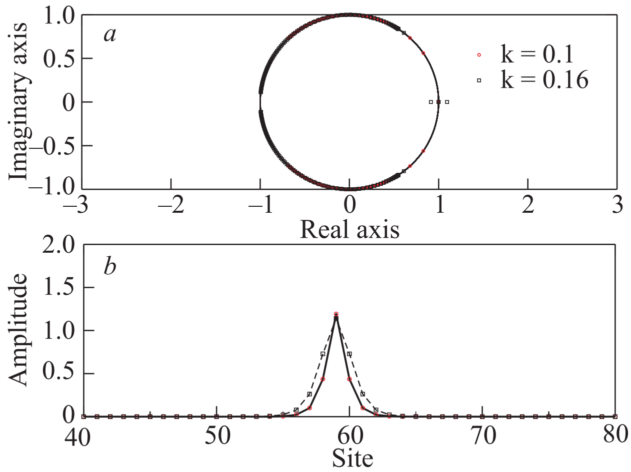

Fig. 1. Floquet eigenvalues of DB solutions with frequency $\omega_b = 0.863$, and coupling $k = 0.1$ (circles) and coupling $k = 0.16$ (squares) (*a*). Oscillator amplitudes for the DB as a function of lattice sites for $k = 0.1$ (circles with solid line) and $k = 0.16$ (squares with dashed line) (*b*).

Figure 2 contains more information on the linear stability of DBs. Denoting a Floquet eigenvalue by $\lambda = \rho e^{i\theta}$, we measure θ — the eigenvalue's angle

$$\theta = \arctan\left(\frac{\mathrm{Im}\,(\lambda)}{\mathrm{Re}\,(\lambda)}\right), \text{ and } \rho = |\lambda| = \sqrt{\mathrm{Re}\,(\lambda)^2 + \mathrm{Im}\,(\lambda)^2}$$

— its absolute value (upper and lower panel of Fig. 2 as a function of coupling respectively).

For coupling $k < 0.15$ all eigenvalues are located on the unit circle, and the DB is stable. Small perturbations stay small. Moreover, the two continuous arcs do not overlap. Therefore an incoming small amplitude plane wave does not interact with other plane waves, and is elastically scattered by the DB [24]. Thus, we expect that a thermal background will have a rather weak impact on the DB evolution.

For coupling $k \approx 0.15$ two eigenvalues from the discrete spectrum part leave the unit circle, and an instability occurs. The corresponding Floquet eigenvector is localized around the DB, therefore that instability is a local one. Small perturbations will therefore enforce the DB to change in time. However, the two continuous arcs are still not overlapping, and the plane wave scattering is still elastic in this case [24]. Therefore the DB should not gain or loose energy on average. We expect that it will therefore not disappear in the presence of thermal noise.

Increasing the coupling beyond $k = 0.169$, a sequence of instabilities with respect to extended perturbations appears due to the overlap of the two continuous arcs. These instabilities are characterized by small deviations of the corresponding Floquet eigenvalues from the unit circle, which are of the order of the inverse system size [25].

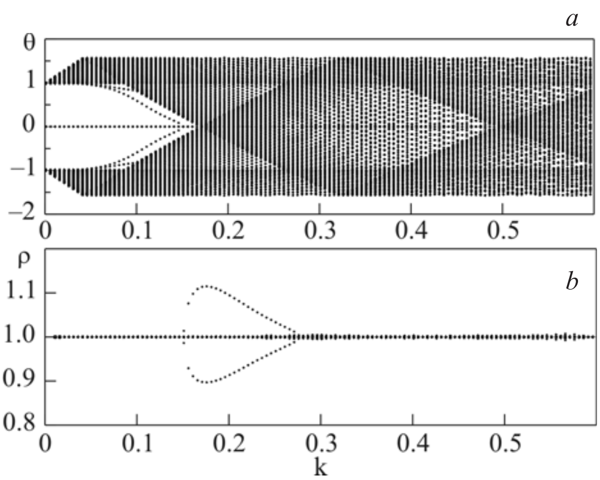

Fig. 2. θ as a function of coupling k (*a*). ρ as a function of coupling k (DB of frequency $\omega = 0.863$) (*b*).

Therefore one would expect, that these instabilities do not matter for large systems. However, in their presence, the scattering of a plane wave is drastically changed from elastic to inelastic [24]. Moreover, the scattering is happening on the expense of the DB energy [24]. We expect therefore, that these DBs will dissolve much faster into a thermal background.

3. Thermal fluctuations and DBs

3.1. Methods

In order to study the interaction between the breather and the thermal environment we proceed as follows. The lattice size is now $N = 4000$. We prepare a thermalized environment using Langevin dynamics. We add a damping term $-\gamma \dot{x}_i$ in the right hand side of Eq. (1) as well as a white noise ξ with correlation function $<\xi(t)\xi(t')> = 2\gamma T \delta(t-t')$, where $\gamma = 0.01$ is the damping constant, and $T = 0.005$ is the temperature. We integrate the system for 2000 time units ($0 \le t \le 2000$) and then remove the two terms (damping and white noise) and excite a DB in the center of the lattice. During that second period $2000 \le t \le 14000$ we compute several quantities, e.g. the energy density evolution, and the time dependence of the energy stored in a finite volume around the DB excitation center. We consider DBs with different stability properties (see previous section). The frequency of all DBs is $\omega_b = 0.863$.

Denote the total energy of the system by $\mathcal{E}$ and the energy per particle $E = \mathcal{E}/N$. The energy per particle is reaching the value $E \approx T = 0.005$ at the end of the thermalization process ($t = 2000$), see Fig. 3. During the second period ($t > 2000$), where the breather is added into the lattice, the total energy $\mathcal{E}$ of the system, and therefore also the energy per particle E, are strictly constant during the remaining simulation, see Fig. 3.

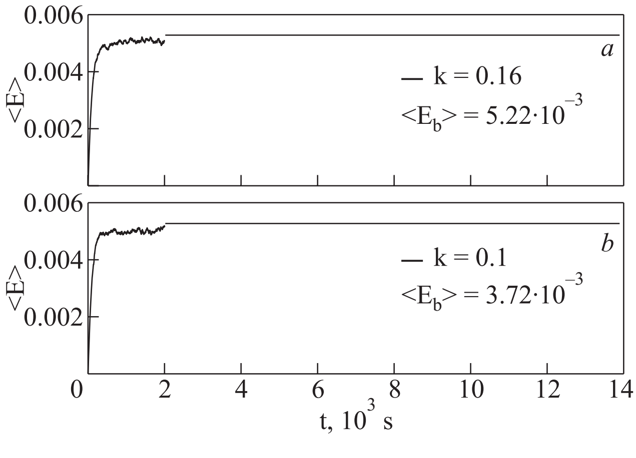

Fig. 3. The energy per particle E versus time. We run the equations of motion with Langevin dynamics for the first 2000 time units and then integrate the Hamiltonian system for the rest of the time (upper panel for $k = 0.16$, lower panel $k = 0.1$). The values for the DB energy per particle E_b are 0.00522 and 0.00372, correspondingly.

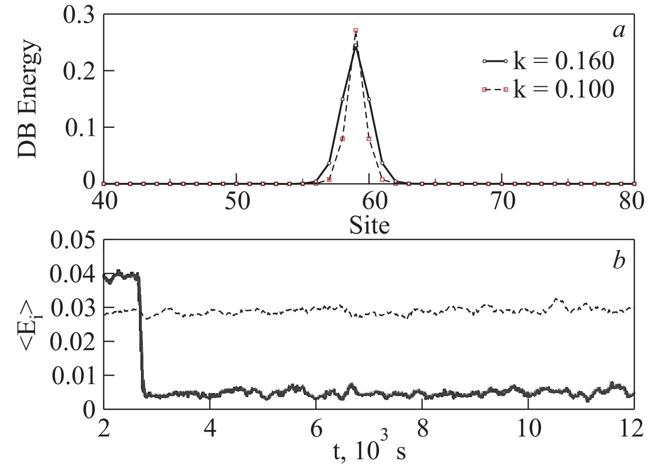

Fig. 4. The energy distribution within the DB, $k = 0.16$ — circles with solid line, $k = 0.1$ — squares with dashed line) (*a*). The energy stored in 21 sites around the position of the DB excitation as a function of time i.e. $< E_i > = (1/21)\sum_{i=n/2-10}^{n/2+10} E_i$, ($k = 0.16$ solid line, and $k = 0.1$ dashed line) (*b*).

3.2. Stable discrete breathers

We start with $k = 0.1$, which corresponds to a stable DB solution (dashed line in Fig. 4,*a*). We measure the energy stored in 21 sites around the DB position during the second period (dashed line, Fig. 4,*b*). We find no significant change in time. Therefore, the DB does not dissolve, and does not leave the finite volume. Indeed, the evolution of the energy density during the second period is shown in Fig. 5,*b*. We observe, that the DB does not undergo significant changes.

3.3. Unstable discrete breathers

3.3.1. Instability due to local perturbations. We repeat the above study for $k = 0.16$. Now the DB is unstable with respect to local perturbations. At the same time it is still elastically scattering plane waves. The energy stored in a finite volume around the DB excitation position is sharply decreasing around $t \approx 2800$ (solid line, Fig. 4,*b*). Checking the evolution of the energy density in Fig. 5,*a*, wobserve that the DB starts moving through the lattice, but does not dissolve, in accord with our expectations.

3.3.2. Instability due to extended perturbations. We continue wuth the cases $k = 0.3$ and $k = 0.4$. According to Fig. 2 the two continuous arcs overlap, and therefore DBs are unstable with respect to extended perturbations. Yet the deviation of the Floquet eigenvalues from the unit circle is small — of the order of the inverse system size, which in our case amounts to 0.00025. The characteristic times on which such instabilities could show up are of the

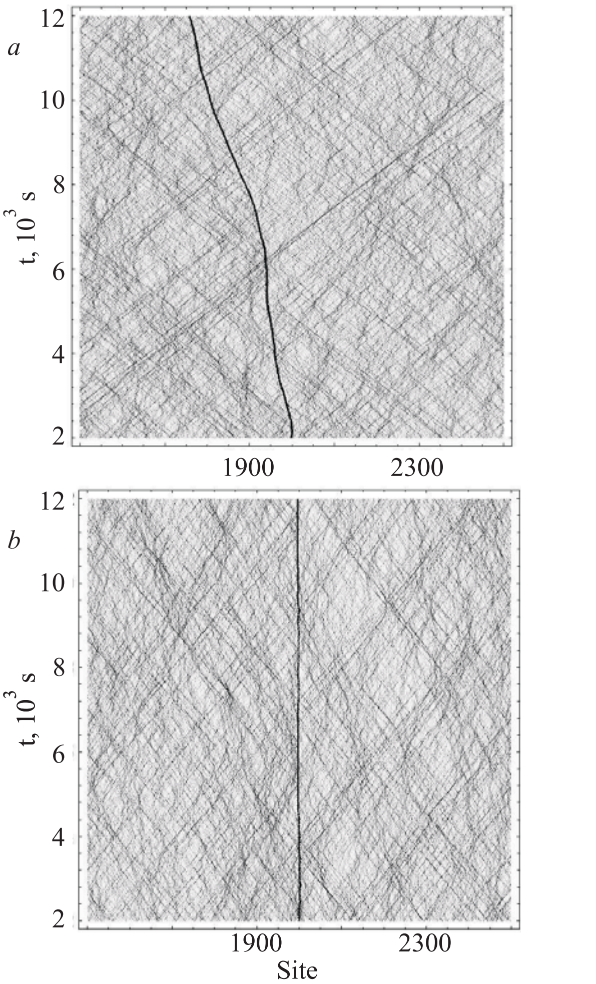

Fig. 5. Energy density plots: DB of $k = 0.16$ (*a*), DB of $k = 0.1$ (*b*). In the horizontal axis are the lattice sites (zoom around the central site $i = 2000$ while in the vertical axis is the time). The lattice size is $N = 4000$. The black color indicates the sites with higher energy.

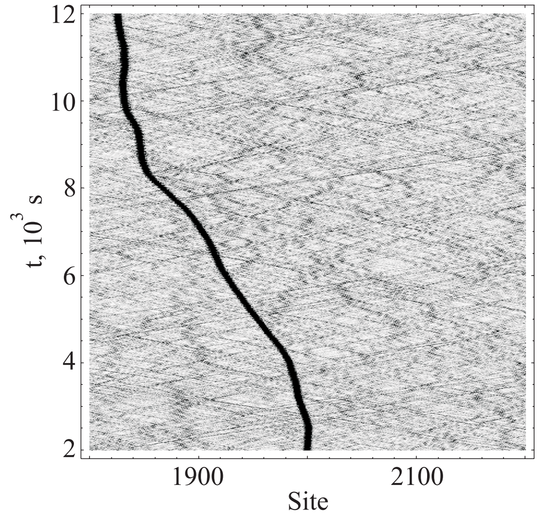

Fig. 7. Energy density plot for $k = 0.3$. In the horizontal axis are the lattice sites (zoom around the central site $i = 2000$ while in the vertical axis is the time). The lattice size is $N = 4000$. The black color indicates the sites with higher energy.

order of 4000 — well inside the time window of our computational studies. We remind the reader, that in these cases the scattering of plane waves by the DB is inelastic, and going on the expense of the DB. In Ref. 24 a monochromatic wave was sent onto such an unstable DB, and the outcome was, that due to slow energy loss the DB unpins and starts to slide through the lattice, without much further loss of its energy.

In Fig. 6 we show the DB profile for $k = 0.3$, and the time dependence of the energy stored in a finite volume around the initial DB excitation. At variance to the case $k = 0.16$, we observe a two-step process. First the energy is decreasing slowly, and around $t = 3200$ it rapidly decreases down to the thermal background average. In Fig. 7 we show the corresponding energy density plot,

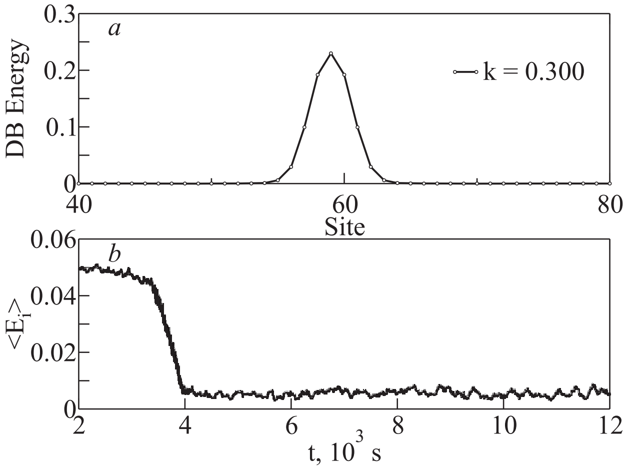

Fig. 6. The energy distribution within the DB for $k = 0.3$ (*a*). The energy stored in 21 sites around the position of the DB excitation as a function of time $< E_i > = (1/21)\sum_{i=n/2-10}^{n/2+10} E_i$ (*b*).

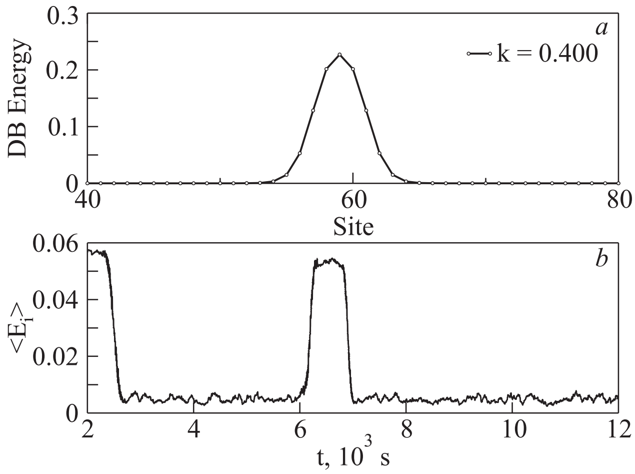

Fig. 8. The energy distribution within the DB for $k = 0.4$ (*a*). The energy stored in 21 sites around the position of the DB excitation as a function of time $< E_i > = (1/21)\sum_{i=n/2-10}^{n/2+10} E_i$ (*b*).

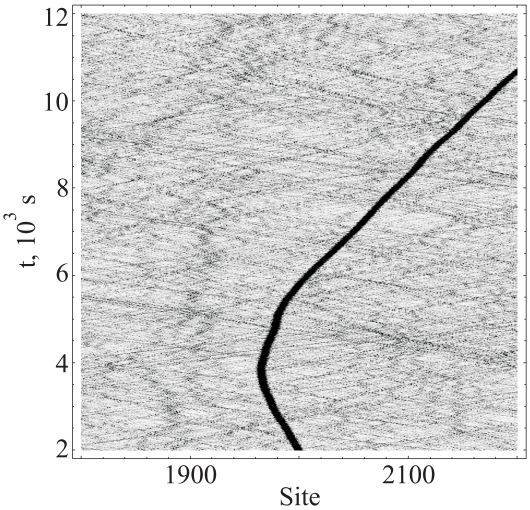

Fig. 9. Energy density plot for $k = 0.4$. In the horizontal axis are the lattice sites (zoom around the central site $i = 2000$ while in the vertical axis is the time). The lattice size is $N = 4000$. The black color indicates the sites with higher energy.

which shows, that the DB starts to move around the time $t = 3200$, but does not dissolve. Therefore we conclude, that during the first time period $t \leq 3200$ the DB is not moving, but slowly decreasing its energy due to inelastic scattering of plane waves. After that first period, the DB starts to move in the lattice, similar to the observation in Ref. 24.

We repeat the computations for $k = 0.4$. In Fig. 8 the energy stored in the finite volume around the initial DB excitation is shown. It rapidly decreases, but then increases again for a short period. Note that during that second splash, the energy maximum energy is lower than the initial value. Therefore the DB is starting to move, but changes it direction of motion, and passes through the original excitation site again at a later time. At the same time it has been inelastically scattering plane waves, and lost some energy during that process. Indeed, the energy density plot in Fig. 9 confirms these conclusions.

4. Discussion

We have shown, that the interaction between a DB and a thermal background depends strongly on the stability properties of DBs, and on the related properties of elastic or inelastic plane wave scattering. Therefore, we may expect that long-lived pinned DB excitations in thermal equilibrium will be excited, if the corresponding DB is stable. Moving DB-like excitations will be excited, if the corresponding DB is locally unstable. The corresponding energies of the DB solutions will yield Boltzmann probability factors, which will tell the probability of randomly creating such an excitation. Finally, DB solutions with overlapping continuous arcs of their Floquet spectrum inelastically scatter waves, on the expense of their DB energy. Nevertheless even these DB excitations survive the interaction with a thermal background without much loss, while moving erratically through the lattice, and only slowly reduce their energy.

This work is dedicated to the memory of Arnold Markovich Kosevich. His early contributions in the field of discrete breathers have been of great importance for further progress in the subject. Arnold Markovich's continued interest in that field, over decades, was very important, and stimulated and motivated the interest of especially young researchers in this rapidly evolving area of nonlinear dynamics and physics of complex systems.

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