Unusual slow energy relaxation induced by mobile discrete breathers in one-dimensional lattices with next-nearest-neighbor coupling

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Abstract

We study the energy relaxation process in one-dimensional (1D) lattices with next-nearest-neighbor (NNN) couplings. This relaxation is produced by adding damping (absorbing conditions) to the boundary (free-end) of the lattice. Compared to the 1D lattices with on-site potentials, the properties of discrete breathers (DBs) that are spatially localized intrinsic modes are quite unusual with the NNN couplings included, i.e. these DBs are mobile, and thus they can interact with both the phonons and the boundaries of the lattice. For the interparticle interactions of harmonic and Fermi–Pasta–Ulam–Tsingou–β (FPUT–β) types, we find two crossovers of relaxation in general, i.e. a first crossover from the stretched-exponential to the regular exponential relaxation occurring in a short timescale, and a further crossover from the exponential to the power-law relaxation taking place in a long timescale. The first and second relaxations are universal, but the final power-law relaxation is strongly influenced by the properties of DBs, e.g. the scattering processes of DBs with phonons and boundaries in the FPUT–β type systems make the power-law decay relatively faster than that in the counterparts of the harmonic type systems under the same coupling. Our results present new information and insights for understanding the slow energy relaxation in cooling the lattices.

Keywords: energy relaxation, discrete breathers, next-nearest-neighbor coupling

(Some figures may appear in colour only in the online journal)

1. Introduction

Discrete breathers (DBs), also known as intrinsic localized modes, are spatially localized nonlinear vibrational modes in defect-free discrete systems. In the past decades, huge numbers of theoretical and experimental studies had been devoted to confirming the existence and stability of DBs. Most of the theoretical studies focused on the anharmonic chains at zero temperature, from which the existence of DBs has been proved exactly (see [1, 2] and reviews [3, 4]). Since then, in other periodic systems such as cantilever arrays [5], Josephson junction arrays [6, 7], electrical lattices [8, 9], mass-spring chains [10], arrays of coupled pendula [11], chains of magnetic pendulums [12], and granular crystals [13, 14], the existence of DBs has been proved experimentally. There are also many studies in real crystals [15], for example, in ionic NaI [16], covalent Si, Ge, and diamond [17, 18], α-uranium [19], ordered alloys [20] as well as proteins [21, 22].

Standing DBs are localized modes of system energy. However, sometimes DBs can move with a small velocity. These mobile excitations can thus interact with the boundaries. It is thus interesting to study how this kind of DBs...
affects the energy relaxation at a finite-temperature system when the boundaries play a role. By using the cooling method, i.e. imposing the absorbing conditions on the boundaries, Aubry and Tsiron [23] first observed the stretched-exponential lattice energy relaxation induced by standing DBs in one-dimensional (1D) lattices with on-site potentials, in contrast to the standard exponential relaxation law of the corresponding linear chains. Subsequently, the counterpart two-dimensional lattices have been considered and a similar conclusion has been drawn in [24]. Further detailed studies [25, 26] of the harmonic and anharmonic chains without on-site potentials showed that the stretched-exponential energy relaxation is not universal, instead a usual exponential relaxation law is observed in a short time, followed by a power-law decay over a long time. The mechanism of the change of the power-law relaxation is induced by standing DBs. As the interactions of standing DBs with the boundaries are very weak, the energy release is actually suppressed and it is thus difficult to observe equilibrium states on typical simulation time scales. As a result, the lattice is in a metastable state, called the nonequilibrium residual state, similar to the glassy patterns in disordered systems.

In addition to the above progress, it would be worth noting that the properties of DBs have been found to be related to other physical properties. For example, by considering some complex crystal structures, such as the next-nearest-neighbor (NNN) interactions [27, 28], the lattice with altering mass or interactions [29], the on-site potentials [30–32] and the long-rang interactions [33], DBs have been studied in the perspective of energy transport. In such cases, DBs are more evident and sometimes can be moveable. This causes these kinds of DBs to be effective scatterers of both phonons and boundaries [34], hence they can reduce the thermal conductivity [32, 33]. We also note that even only considering the role of nonlinearity, DBs can already affect some other macroscopic properties [35], e.g. elastic constants [36], thermal expansion [37, 38], and heat capacity [36, 38, 39].

The purpose of this paper is to study slow energy relaxation in a more complicated situation including mobile DBs. To this end, we shall focus on the Fermi–Pasta–Ulam–Tsingou–β (FPUT-β) chain with NNN interactions. By properly adjusting the ratio of the NNN coupling to the nearest-neighbor (NN) coupling, one might be able to produce the mobile DBs [27, 28]. Therefore, by employing such models we are devoted to exploring the combined effects of NNN interactions and nonlinearity (which produces moveable DBs) on the slow energy relaxation. The rest of this article is organized as follows: In section 2 we describe the reference models; section 3 presents the cooling methods to study energy relaxation and the physical quantities of interest; section 4 provides the main results for different lattice models, from which the role of NNN interactions and nonlinearity will be demonstrated; Finally, section 5 draws our conclusion.

2. Models

A general 1D lattice with both NN and NNN interparticle interactions and without on-site potential can be represented by

\[ H = \sum_{l} \left[ \frac{p_i^2}{2} + V(x_{i+1} - x_i) + \gamma V(x_{i+2} - x_i) \right], \]

where \( p_i \) is the \( i \)th (totally \( N \) particles and all with unit mass) particle’s momentum, \( x_i \) is its displacement from the equilibrium position, \( V(\xi) \) is the interparticle potential and the parameter \( \gamma \) specifies the comparative strength of the NNN to NN couplings. We use the FPUT-β interparticle interaction \( V(\xi) = \frac{1}{2} \xi^2 + \frac{1}{4} \xi^4 \) to mainly consider the combined role of NNN coupling and nonlinearity in energy relaxation. For such a model, it would be worth noting that it has a special phonon dispersion relation (see Figure 1 for the phonon spectrum):

\[ \omega_q = 2\sqrt[3]{\sin^2(q/2) + \gamma \sin^2 q}, \]

where \( q \) is the wave number for phonons and \( \omega_q \) is the corresponding frequency. From this dispersion relation, one obtains the phonons’ group velocity \( v_g = d\omega_q/dq = \omega^{-1}[\sin q + \gamma \sin(2q)] \) and finds that: (i) for \( 0 < \gamma < 0.25, v_g > 1 \), which is in contrast to \( v_g = 1 \) in the case of systems with NN coupling; (ii) for \( \gamma = 0.25, v_g \) is very close to zero in a wider \( k \) domain near the Brillouin zone boundary; (iii) for \( \gamma > 0.25, \) both \( v_q \) and \( v_g \) are actually degenerate, i.e. one \( \omega_q/v_g \) corresponds to two \( q \) values. These unusual properties can favor the formation of a special highly moving localized excitation (mobile DBs) in the presence of appropriate nonlinearity [27, 28] and thus one can expect that such properties would greatly influence the energy relaxation.

3. Method

We use the cooling method to reveal the slow energy relaxation and to obtain the information of DBs. For this purpose, we first thermalize the lattices to a fixed temperature \( T = 0.1 \) by using the Nose–Hoover [40] heat baths. Then after

![Figure 1](image-url)
the systems are fully thermalized for a considerably long time, we remove the heat baths and add the absorbing boundary conditions. That is to say, we impose damping to both ends (which are free) of the lattices, and so the equation of motion of the system can be expressed by

\[ x_i = V'(x_{i+1} - x_i) + V'(x_i - x_{i-1}) + \gamma V'(x_{i+2} - x_i) + \gamma V'(x_i - x_{i-2}) - \eta \frac{\delta (\partial^2 x_i + \delta_{i,N})}{\delta t^2}. \]

(2)

Here \( \dot{x}_i = \frac{d}{d\xi} \), \( V'(\xi) \) represents \( \frac{\delta V}{\delta x} \), \( \eta \) is the dissipation exponent and we fix \( \eta = 0.1 \) in practice; \( \delta \) is the Kronecker delta.

By performing the cooling method, we are interested in the decay of the total energy. To reveal this decay, we first define the symmetrized site energies:

\[ h_i = \frac{1}{2} \dot{\xi}_i^2 + \frac{1}{2} [V(x_{i+1} - x_i) + V(x_i - x_{i-1}) + \gamma V(x_{i+2} - x_i) + \gamma V(x_i - x_{i-2})]. \]

(3)

With such a definition, the total energy of the system is given by \( E = \sum_{i=1}^{N} h_i \). We can now study the decay of the normalized energy \( E(t)/E(0) \), which represents the ratio of the decayed energy to the initial energy. As it has been shown that in some cases the exponential law or the stretched-exponential law is observed. To identify what exactly the law is, it is better to plot

\[ D(t) = -\ln \left( \frac{E(t)}{E(0)} \right). \]

(4)

We remind readers that since the energy localization might be strongly inhibited by fixed-end boundary conditions [25, 26], in our simulations we apply the free-end boundary conditions. The motion equations are integrated with the velocity-Verlet algorithm [41] with a time step 0.01. With both heat baths and damping, the systems are first evolved \( 10^6 \) times with the heat baths to reach the stationary state under the given temperature, and then evolved additional \( 10^6 \) times without the heat baths but with the damping presented, which enables us to reveal the relaxation process induced by the absorbing boundaries.

4. Results

4.1. Harmonic system

To show the role of NNN coupling in slow energy relaxation separately, let us first check the results of the relevant linear systems with NNN coupling. For the same harmonic system with the NN coupling only, it has been theoretically predicted that [25]

\[ \frac{E(t)}{E(0)} = \begin{cases} e^{-t/\tau_0} & \text{for } t \ll \tau_0, \\ \left[ \frac{2\pi(t/\tau_0)^2}{\pi(t/\tau_0)} \right]^{-1/2} & \text{for } t \gg \tau_0. \end{cases} \]

(5)

This means that one generally finds two energy relaxation processes, i.e. the exponential law and the inverse-square-root law, for short and long timescales, respectively. Such two laws have been verified in a harmonic chain with NN coupling only under a small \( N = 32 \), but some deviations have also been numerically observed [25, 26], i.e. a new exponential relaxation recovers in a longer time. In view of this, we study the dependence of the energy relaxation properties on \( \gamma \) here in a large system size \( N = 4096 \) in figure 2(a). Surprisingly, in a time of \( t < 10^4 \), regardless of \( \gamma \), the results of \( D \) versus \( t \) follow two general power-laws (\( \sim t^\mu \)) with \( \mu = 0.68 \) and \( \mu = 1.03 \), respectively. This suggests that in addition to the previously theoretically predicted exponential law, there is another stretched-exponential law \( e^{-t^\gamma/\xi} \) with \( \nu = 0.68 \) at a shorter time, independent of the NNN coupling ratio \( \gamma \). Figure 2(a) also suggests that the long-time behavior of the energy relaxation should depend on \( \gamma \). To see this more explicitly, figure 2(b) depicts the results of \( E(t)/E(0) \) versus \( t \) in harmonic systems with NNN coupling. A log–log plot then helps us clearly identify several power-law exponents. The best fittings give \( E(t)/E(0) \sim t^{-\nu} \) with \( \nu = 0.54, \mu = 0.52, \mu = 0.16 \), and \( \mu = 0.13 \) for \( \gamma = 0, \gamma = 0.025, \gamma = 0.25 \), and \( \gamma = 0.4 \), respectively (in a long time). It indicates that including the NNN coupling seems to further slow down the energy relaxation process. This is not trivial since from figure 1 by including the NNN coupling, on one hand the phonon group velocity \( v_g \) is increased with the increase of \( \gamma \). This speeds up the energy relaxation process. On the other hand, the increase of \( \gamma \) causes more phonons with higher frequencies to emerge, which however slows down the relaxation. Therefore, in a linear system with NNN coupling but without nonlinearity and DBs, the overall effect is to depress the energy relaxation process during the cooling.

4.2. FPUT-\( \beta \) system

With the above understanding, let us now consider the combined effects of NNN coupling and nonlinearity. For this purpose, as mentioned we focus on the popular 1D FPUT-\( \beta \) lattice. Figure 1(c) shows that the first stretched-exponential and exponential laws of \( E(t)/E(0) \) for \( t < 10^4 \), which are similar to that shown in figure 1(a). Therefore, these two relaxation laws seem independent of the NNN coupling, even when one includes the nonlinearity in the systems. This may also suggest that such two laws for \( t < 10^4 \) are general, at least for both the linear and nonlinear systems with NNN coupling. Therefore, the origin of this finding is worth studying in the future.

Again, the distinctions for different \( \gamma \) in the FPUT-\( \beta \) systems still lie in the long-time behavior. As can be seen in figure 2(d), \( E(t)/E(0) \) follows a \( t^{-\mu} \) law at long timescales, similar to those observed in the harmonic systems as shown in figure 2(b). A further comparison of figures 2(b) and (d) shows that the power-law exponent \( \mu \) for harmonic and FPUT-\( \beta \) systems under the same \( \gamma \) is different, i.e. \( \mu \) for the FPUT-\( \beta \) lattice is larger than that for harmonic lattice as long as \( \gamma = 0 \). It presents a clue that the combined effects of NNN coupling and nonlinearity seem to speed up the relaxation during the cooling.

In order to have a close look at this trend, in figure 3 we plot \( \mu \) against \( \gamma \) for both the harmonic and FPUT-\( \beta \) lattices. Therein four data points are extracted from figures 2(b) and (d), while others are calculated additionally in the same way.
Indeed, in the range of $\gamma$ investigated, all $\mu$ of FPUT-$\beta$ systems are larger than those of the harmonic systems. Indeed, this indicates that the combined effects of the NNN coupling and nonlinearity are to make the energy relaxation relatively faster if compared with the counterpart linear systems.

4.3. The origin of the relatively faster energy relaxation: the role of mobile DBs

We lastly explain the observed relatively faster energy relaxation in a nonlinear system compared to the counterpart linear systems. As it has already been pointed out in the introduction, the slow energy relaxation behaviors in nonlinear lattices are usually related to the energy localization and these localization origins from the excitation of standing DBs. In the absence of nonlinearity, it was previously regarded that the energy relaxation will turn back to the traditional exponential decay \[25\]. However, our above results in figure 2 suggest that even for linear systems, this is not the case. The long-time behavior of the energy relaxation seems always to be a power-law decay. Combining the results of linear and nonlinear systems (see figures 2(a)–(d)), one might conclude that the power-law energy relaxation in a long time is general but the details of the power-law exponent are then affected by the localization induced by DBs. To illustrate this point, in figure 4 we plot a snapshot of the lattice displacements at the end of the simulation, i.e. by imposing the damping to both harmonic and FPUT-$\beta$ systems after a time $10^6$ (with $\gamma = 0.25$ for an example). As can be seen, only in the FPUT-$\beta$ system do we identify the emergence of DBs (see the inset of figure 4(b), a profile of DBs can be found there), which is in clear contrast to that observed in the harmonic system (see the inset of figure 4(a)).

Since DBs can localize energies, one may wonder why the energy relaxation in the nonlinear systems with NNN coupling is relatively faster than that in the counterpart linear systems. This can be understood from figure 5 if we further examine the mobility of DBs. In figure 5 we plot the same snapshot of the lattice displacements after imposing the damping of the free-end boundaries of the nonlinear lattice ($\gamma = 0.25$) for four long times. It can be seen that due to the mobility of DBs, they can interact with both phonons and boundaries, which produces an additional passageway for speeding up the energy relaxation. This is surely different...
from the main passageway of phonons-boundaries scattering as shown in the relevant linear model (see figure 4(a)).

5. Conclusion

To summarize, by applying a damping term into the system’s boundaries, we have numerically studied the energy relaxation processes in both 1D linear and FPUT-β lattices when the NNN interactions are considered. As we expect that including the NNN coupling might need a longer time for systems to relax, we have considered a system size much larger than that that was taken into account of in previous studies. For both linear and nonlinear lattices, generally the short-time ($t < 10^4$) relaxation behaviors are given by a stretched-exponential law, followed by an exponential law, which is independent of the ratio of the NNN coupling. This justifies that even linear systems can also support the stretched-exponential relaxation law at some timescales. Furthermore, the long-time ($t > 10^4$) behavior is however determined by a power-law with the
exponent strongly dependent on $\gamma$, i.e. as $\gamma$ increases, the relaxation is slowed down. This means that including the NNN coupling makes the long-time power-law energy relaxation slower. Further introducing the nonlinearity, however, in turn, speed up the relaxation, which is induced by the emergence of mobile DBs. These mobile DBs can interact with both phonons and boundaries, which then produce an additional passageway for scattering the energies. Finally, this novel energy relaxation behavior, induced by mobile DBs in the nonlinear lattices with NNN coupling, is surely different from the stretched-exponential relaxation observed in lattices with on-site potentials that are mainly produced by the standing DBs [23, 24].

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References

[1] Sievers A J and Takeno S 1988 Intrinsic localized modes in anharmonic crystals Phys. Rev. Lett. 1 970
[2] Page J B 1990 Asymptotic solutions for localized vibrational modes in strongly anharmonic periodic systems Phys. Rev. B 41 7835
[3] Flach S and Willis C R 1998 Discrete breathers Phys. Rep. 295 181
[4] Flach S and Gorbach A V 2008 Discrete breathers—advances in theory and applications Phys. Rep. 467 1
[5] Sato M, Hubbard B E and Sievers A J 2006 Colloquium: Nonlinear energy localization and its manipulation in micromechanical oscillator arrays Rev. Mod. Phys. 78 137
[6] Tria E, Mazo J J and Orlando T P 2000 Discrete breathers in nonlinear lattices: experimental detection in a Josephson array Phys. Rev. Lett. 84 741
[7] Binder P, Abraimov D, Ustinov A V, Flach S and Zolotaryuk Y 2000 Observation of breathers in Josephson ladders Phys. Rev. Lett. 84 745
[8] Palmero F, English L Q, Chen X-L, Li W, Cuevas Maraver J and Kevrekidis P G 2019 Experimental and numerical observation of dark and bright breathers in the band gap of a diatomic electrical lattice Phys. Rev. E 99 032206
[9] Gomez-Rojas A and Halevi P 2018 Discrete breathers in an electric lattice with an impurity: birth, interaction, and death Phys. Rev. E 97 022225
[10] Watanabe Y, Nishida T, Doi Y and Sugimoto N 2018 Experimental demonstration of excitation and propagation of intrinsic localized modes in a mass–spring chain Phys. Lett. A 382 1957
[11] Cuevas J, English L Q, Kevrekidis P G and Anderson M 2009 Discrete breathers in a forced-damped array of coupled pendula: modeling, computation, and experiment Phys. Rev. Lett. 102 224101
[12] Russell F M, Zolotaryuk Y, Eilbeck J C and Dauxois T 1997 Moving breathers in a chain of magnetic pendulums Phys. Rev. B 55 6304
[13] Voronnikov K, Starosvetsky Y, Theocharis G and Kevrekidis P G 2018 Wave propagation in a strongly nonlinear locally resonant granular crystal Physica D 365 27
[14] Chong C, Porter M A, Kevrekidis P G and Daraio C 2017 Nonlinear coherent structures in granular crystals J. Phys.: Condens. Matter. 29 413003
[15] Dmitriev S V, Korznikova E A, Baimova J A and Velarde M G 2016 Discrete breathers in crystals Phys. Usp. 59 446
[16] Khadeeva L Z and Dmitriev S V 2010 Discrete breathers in crystals with NaCl structure Phys. Rev. B 81 214306
[17] Riviere A, Lepri S, Colognesi D and Piazza F 2019 Wavelet imaging of transient energy localization in nonlinear systems at thermal equilibrium: the case study of NaI crystals at high temperature Phys. Rev. B 99 024307
[18] Murzaev R T, Bachurin D V, Korznikova E A and Dmitriev S V 2017 Localized vibrational modes in diamond Phys. Lett. A. 381 1003
[19] Murzaev R T, Babicheva R I, Zhou K, Korznikova E A, Fomin S Y, Dubinko V I and Dmitriev S V 2016 Discrete breathers in alpha-uranium Eur. Phys. J. B 89 168
[20] Dubinko V, Laptev D, Terentyev D, Dmitriev S V and Irwin K 2019 Assessment of discrete breathers in the metallic hydrides Comp. Mater. Sci. 158 389
[21] Juanico B, Sanejouand Y-H, Piazza F and De Los Rios P 2007 Discrete breathers in nonlinear network models of proteins Phys. Rev. Lett. 99 238104
[22] Gnizanlong C L, Ndjomatchoua F T and Tchawoua C 2020 Forward and backward propagating breathers in a DNA model with dipole-dipole long-range interactions Phys. Rev. E 102 052212
[23] Tsironis G P and Aubry S 1996 Slow relaxation phenomena induced by breathers in nonlinear lattices Phys. Rev. Lett. 77 5225
[24] Bikaki A, Voulgarakis N K, Aubry S and Tsironis G P 1999 Energy relaxation in discrete nonlinear lattices Phys. Rev. E 59 1234
[25] Piazza F, Lepri S and Livi R 2001 Slow energy relaxation and localization in 1D lattices J. Phys. A 34 9803
[26] Piazza F, Lepri S and Livi R 2003 Cooling nonlinear lattices toward energy localization Chaos 13 637
[27] Xiong D, Wang J, Zhang Y and Zhao H 2012 Nonuniversal heat conduction of one-dimensional lattices Phys. Rev. E 85 020102
[28] Xiong D, Zhang Y and Zhao H 2014 Temperature dependence of heat conduction in the Fermi-Pasta-Ulam-β lattice with next-nearest-neighbor coupling Phys. Rev. E 90 022217
[29] Xiong D, Zhang Y and Zhao H 2013 Heat transport enhanced by optical phonons in one-dimensional anharmonic lattices with alternating bonds Phys. Rev. E 88 052128
[30] Giardina C, Livi R, Politi A and Vassalli M 2000 Finite thermal conductivity in 1D lattices Phys. Rev. Lett. 84 2144
[31] Gendelman O V and Savin A V 2000 Normal heat conductivity of the one-dimensional lattice with periodic potential of nearest-neighbor interaction Phys. Rev. Lett. 84 2381
[32] Xiong D, Saadatmand D and Dmitriev S V 2017 Crossover from ballistic to normal heat transport in the $\phi^4$ lattice: if nonconservation of momentum is the reason, what is the mechanism? Phys. Rev. E 96 042109
[33] Wang J, Dmitriev S V and Xiong D 2020 Thermal transport in long-range interacting Fermi-Pasta-Ulam chains Phys. Rev. E 102 013179
[34] Saadatmand D, Xiong D, Kuzkin V A, Krivtsov A M, Savin A V and Dmitriev S V 2018 Discrete breathers assist energy transfer to ac-driven nonlinear chains Phys. Rev. E 97 022217
[35] Manley M E 2010 Impact of intrinsic localized modes of atomic motion on materials properties Acta Mater. 58 2926

[36] Korznikova E A, Morkina A Y, Singh M, Krivtsov A M, Kuzkin V A, Gani V A, Bebikho Yu V and Dmitriev S V 2020 Effect of discrete breathers on macroscopic properties of the Fermi-Pasta-Ulam chain Eur. Phys. J. B 93 123

[37] Manley M E, Yethiraj M, Sinn H, Volz H M, Alatas A, Lashley J C, Hults W L, Lander G H, Thoma D J and Smith J L 2007 Intrinsically localized vibrations and the mechanical properties of α-uranium J. Alloy. Compd. 444 129

[38] Mihaila B et al 2006 Pinning frequencies of the collective modes in α-uranium Phys. Rev. Lett. 96 076401

[39] Singh M, Morkina A Y, Korznikova E A, Dubinko V I, Terentiev D A, Xiong D, Naimark O B, Gani V A and Dmitriev S V 2021 Effect of discrete breathers on the specific heat of a nonlinear chain J. Nonlinear Sci. 31 12

[40] Nose S 1984 A unified formulation of the constant temperature molecular dynamics methods J. Chem. Phys. 81 511

Hoover W G 1985 Canonical dynamics: equilibrium phase-space distributions Phys. Rev. A 31 1695

[41] Allen P and Tildesley D L 1987 Computer Simulation of Liquids Clarendon (Clarendon: Oxford)