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SCATTERING OF SMALL-AMPLITUDE PHONONS ON DISCRETE BREATHERS IN FERMI–PASTA–ULAM–TSINGOU CHAIN

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There are two traditionally discussed dispersion relations (DR) in condensed media: gapless phonon DR and DR with an energy or frequency gap. In various fields of condensed matter physics, the third type of DR is of interest, which correspond to gap effects in k-space (Gapped Momentum States – GMS). The growing interest in GMS is associated with important consequences for the dynamic and thermodynamic properties of the system (hydrodynamic turbulence, plasticity, fracture). Traditionally, GMS arise in the Maxwell–Frenkel approach as applied to the viscoelastic properties of liquids and solids, when the DR-gaps can continuously vary from energy to momentum space. This work is the first in a series of studies devoted to the analysis of dispersion effects associated with the anharmonicity of the potential and the emergence of collective breather-type modes, the so-called discrete breathers (DBs), and their influence on the macroscopic properties of nonlinear lattices, for example, on heat conductivity. Recently, the influence of discrete breathers (DBs) on the macroscopic properties of nonlinear lattices, for example, on thermal conductivity has been investigated. When solving this problem, it is important to know how phonons interact with DBs. The scattering of phonon wave packets of small amplitude by standing DBs in the β-Fermi-Pasta-Ulam-Tsingou (β-FPUT) chain is studied numerically for different amplitudes of DBs. It is found that DBs of sufficiently large amplitudes reflect short-wavelength phonons, but remain transparent for long-wavelength phonons. An increase in the DB amplitude expands the reflection region in the short-wavelength part of the first Brillouin zone. These results suggest that DBs in the β-FPUT chain do not strongly affect the thermal conductivity, since heat is transferred mainly by long-wavelength phonons, which are weakly affected by DBs.

Key words: dispersion relations, gap effects, discrete breathers, β-Fermi–Pasta–Ulam–Tsingou chain

1. Introduction

Discrete breathers (DBs) are spatially localized vibrational modes of large amplitude in defect-free nonlinear lattices; they were discovered by mathematicians over three decades ago [1–3]. Extensive studies on DBs are summarised in two reviews [4, 5]. DBs have been experimentally found in arrays of superconducing Josephson junctions [6, 7], in artificial discrete nonlinear systems [8–15], electrical lattices [16, 17], and in crystal lattices [18–25].

The experimental observation of discrete breathers in crystals is not an easy task [18–25], and numerical methods are often used to study them [26–37]. A close relation between DBs and delocalized nonlinear vibrational modes has been demonstrated in [38– 40]. The ultimate goal of studying DBs in crystals [41] is to evaluate their effect on macroscopic properties. It has been demonstrated experimentally in [19, 20] that the presence of DBs affects the heat capacity and thermal expansion of α-uranium. For nonlinear chains the effect of DBs on thermal conductivity [42,43], specific heat [44], thermal expansion and elastic constants was also analyzed in [45].

When studying the effect of DBs on thermal conductivity, it is important to know how phonons are scattered by DBs. It was shown in [42] that with increasing temperature, a transition from ballistic [46] to normal thermal conductivity is observed, and this transition was explained by the excitation of DBs at high temperatures, which effectively scatter phonons and reduce the thermal conductivity.

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The aim of the present work is to analyze the interaction of phonons with DBs in the classical β-Fermi–Pasta–Ulam–Tsingou (β-FPUT) chain [47]. The symmetric anharmonicity, considered in the formulation, makes it possible to avoid the effect of thermal expansion due to the relationship between mechanical and thermal oscillations [48, 49].

The main goal of the work is to study how DBs of different amplitudes affect the propagation of small-amplitude phonons in the β-FPUT chain. The problem of phonon-DB interaction has been considered in [50, 51] and in recent works [52, 53].

DBs can be classified according to the type of anharmonicity: for a soft (hard) type anharmonicity, the DB frequency decreases (increases) with increasing amplitude.

For a chain with a tunable type of anharmonicity, it was shown that in the case of hard-type anharmonicity, DBs are transparent for long-wavelength phonons and reflect short-wavelength phonons, while for the soft-type anharmonicity the opposite effect is observed [53]. In that work, a chain with harmonic coupling and an anharmonic on-site potential was considered. It is interesting to see what happens in the chain without on-site potential, for example, in the β-FPUT chain. In a chain without an on-site potential, the phonon spectrum has no gap and, therefore, only DBs with hard type anharmonicity can exist, since their frequency must be higher than the phonon spectrum. DBs in the FPUT model have been analyzed in [54].

The article presents the mathematical β-FPUT model and simulation setup, discusses the properties of DBs in the β-FPUT chain, , studies the interaction of phonons with DBs, and analizes the results.

2. The model and simulation setup

The dynamics of the β-FPUT chain of particles [47] having mass m is defined by the Hamiltonian

$$H = K + P = \sum_n K_n + \sum_n P_n \,, \tag{1}$$

where K and P are the kinetic and potential energies of the chain, respectively. The kinetic, potential and total energies of particles are

$$K_n = \frac{m\dot{u}_n^2}{2}, \tag{2}$$

$$P_n = \frac{k}{4}\left(u_n - u_{n-1}\right)^2 + \frac{\beta}{8}\left(u_n - u_{n-1}\right)^4 + \frac{k}{4}\left(u_{n+1} - u_n\right)^2 + \frac{\beta}{8}\left(u_{n+1} - u_n\right)^4, \tag{3}$$

$$H_n = K_n + P_n \quad , \tag{4}$$

respectively. Here, the unknown function of time t, $u_n(t)$, is the displacement of the n-th particle from its lattice position, and $\dot{u}_n \equiv du_n/dt$ is its velocity. Each particle interacts with its nearest neighbors through a potential that includes harmonic and anharmonic terms with coefficients k and β, respectively. Using the Hamilton's principle, the following equations of motion can be obtained from (1)–(3):

$$m\ddot{u}_n = k\left(u_{n-1} - 2u_n + u_{n+1}\right) - \beta\left(u_n - u_{n-1}\right)^3 + \beta\left(u_{n+1} - u_n\right)^3. \tag{5}$$

Without loss of generality, we set $h = 1$ for the lattice spacing, $m = 1$, $k = 1$. We also set and investigate the interaction of small-amplitude phonons with DBs of different amplitudes.

A chain of $N = 2^{12} = 2048$ particles with absorbing boundary conditions is considered, so that any radiation from a DB does not affect its dynamics. Small-amplitude phonons, $u_n \sim \exp\left[i\left(2\pi qn/N - \omega_q t\right)\right]$ with wave number $q = 0, 1, ..., N/2$ and frequency ω_q, obey the dispersion relation:

$$\omega_q = 2\sqrt{\frac{k}{m}}\sin\frac{\pi q}{N}, \tag{6}$$

which can be obtained by substituting the phonon solution into the linearized (5) with $\beta = 0$.

Note that the maximal phonon frequency is $\omega_q^{\max} = 2$, which corresponds to $q = N/2$. The phonon group velocity is

$$\upsilon_g = \frac{d\omega_q}{dq} = \frac{2\pi}{N}\sqrt{\frac{k}{m}}\cos\frac{\pi q}{N}. \tag{7}$$

The equations of motion (5) are solved numerically with the help of the symplectic, sixth-order Störmer's method [55] with the time step $\tau = 10^{-3}\sqrt{m/k}$. The total energy of the chain in our simulations is conserved with the relative error not exceeding 10^{-7}.

3. Properties of discrete breathers

For the DBs solution, the following ansatz is used

$$u_n(0) = \frac{(-1)^n A}{\mathrm{ch}\left[\alpha\left(nh - x\right)\right]}, \qquad \dot{u}_n(0) = 0, \tag{8}$$

where A defines DB amplitude, α is the inverse width (degree of localization) of DB, and x is the position of DB. If $x = lh$, where l is an integer, then DB is localized on a particle (on-site DB). For $x = \left(l + 0{,}5\right)h$ the DB is localized in the middle of a bond (inter-site DB).

For the chosen parameters A and x of the ansatz (8), the inverse width of DB is found so that the DB oscillation amplitude A_{DB} is constant in time.

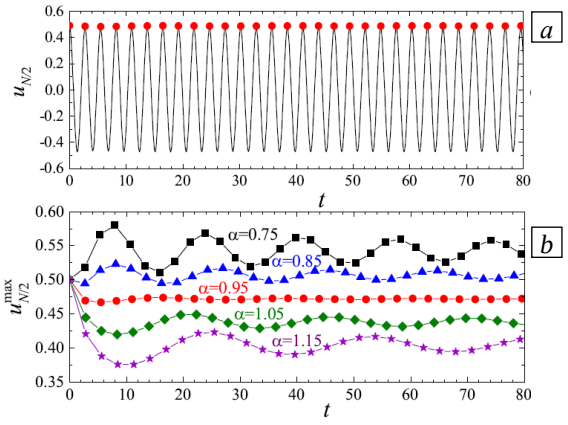

Fig. 1. The displacement of the central particle as the function of time for the on-site DB initiated by the ansatz (8) with $A = 0{,}5$, $x = N/2$ and The red dots mark the maximum points of the curve, that is the DB amplitude $A_{ДБ}$ (b) The maximum points of the curve $u_{N/2}(t)$ for the five values of α, from top to bottom: 0,75, 0,85, 0,95, 1,05, и 1,15 The value α = 0.95 is used in simulations because it produces a DB with minimal oscillation of the amplitude.

An example of fitting the parameter is presented in Fig. 1 for the on-site DB placed in the middle of the chain ($x = N/2 = 1024$) and $A = 0{,}5$. In Fig. 1*a*, the displacement of the DB's central particle

is shown as the function of time for $\alpha = 0,95$. The red dots show the maximal values of $u_{N/2}(t)$, that is the DB amplitude. In Fig. 1*b* the DB amplitude is plotted as the function of time for different values of α from top to bottom: 0.75, 0.85, 0.95, 1.05, and 1.15. It can be seen that for $\alpha = 0.95$, after a transient period of a few DB periods, the DB amplitude becomes time independent, $A_{DB} = 0.472$. This value of α is used for excitation of the DB. It can be seen that even for the best choice of α the DB amplitude is smaller than A, because the ansatz (8) is not an exact breather solution. A part of the energy initially given to the chain is radiated in the form of small-amplitude wave packets moving away from the DB. The wave packets are absorbed at the boundaries and a standing DB remains in the middle of the chain radiating no energy.

In Figs. 2 and 3 one can see properties of the on-site and inter-site DBs, respectively. As the functions of the ansatz parameter A shown are: (a) DB amplitude A_{DB}, DB inverse width α (Fig. 2*a*, *b* (2)), frequency ω (Fig. 2*a*, *b* (3)) and DB energy E (см. Fig. 2*a*, *b* (4)). As mentioned above, A_{DB} is always smaller than A. The DB inverse width increases linearly with A at small amplitudes and then the growth of α with A slows down. The DB frequency bifurcates from the edge of the phonon spectrum (recall that the maximal phonon frequency is ($\omega_q^{\max} = 2$) and increases with A due to the hard type anharmonicity ($\beta > 0$) of the considered chain.

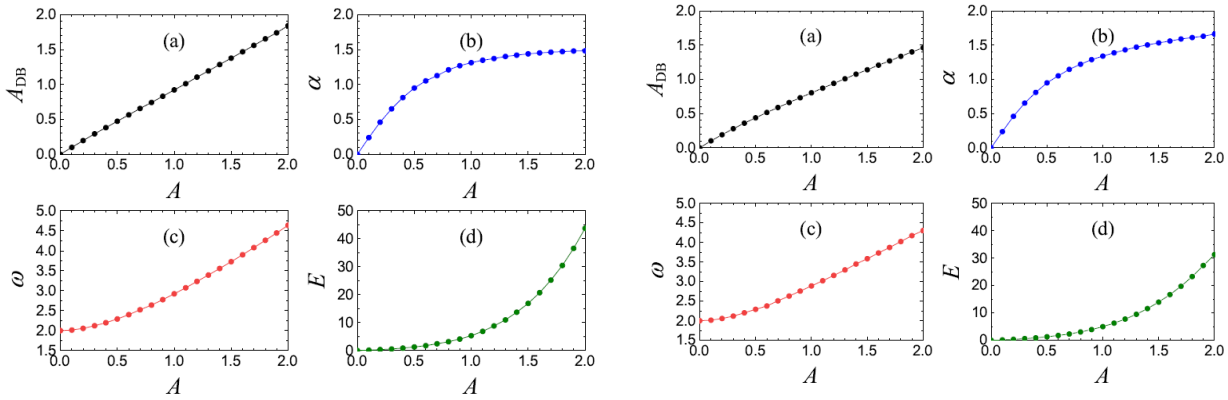

Fig. 2. The parameters of the on-site DB as the functions of the parameter A_{DB} : of the ansatz (8): (a) DB amplitude, (b) inverse width, (c) frequency, and (d) energy.

4. Phonon scattering on DB

Let us proceed to the numerical analysis of the interaction of low-amplitude phonon wave packets with DBs. In doing so, we place a DB in the middle of a chain of $N = 2048$ particles by setting ($x = N/2$) in (8) and excite a phonon wave packet moving to the right in the left half of the chain:

$$u_n(t) = e\sin\left(\frac{2q\pi n}{N} - \omega_q t\right), \quad 0 \le n \le N/2 - s,$$
$$u_n(t) = 0, \quad N/2 - s < n < N, \tag{9}$$

where e, q and ω_q are the phonon amplitude, wavenumber, and frequency, respectively. We set $s = 10$ in (9) to ensure that initially the phonon does not overlap with the DB. Phonons with different wavenumbers q are considered. Recall that the relation between q and ω_q is established by (6). The phonon amplitude is chosen very small, $e = 3\times10^{-4}$, in order to minimize the effect of the phonon on the discrete breather.

According to the results reported by Flach and Gorbach [54], the on-site DB is unstable, and for this reason, the scattering of phonons is studied only on the inter-site DB. The phonon wavepacket

propagates towards the DB and is partly reflected and partly transmitted. The transmission coefficient is defined as follows:

$$e_t = E_t / E_0 , \tag{10}$$

where E_t is the phonon energy per particle transmitted through the DB and $E_0 = e^2 \omega_q^2 / 2$ is the incident phonon energy per particle.

The transmission coefficient as the function of the normalized phonon wavenumer is plotted in Fig. 3 for different values of DB amplitude. It is seen that for $A_{DB} < 0.5$ the DB is practically transparent for all phonons in the first Brillouin zone, since e_t is close to unity. With an increase in $A_{ДБ}$, the transmission coefficient decreases, and the most noticeable decrease is observed for short-wavelength phonons. For not very large A_{DB}, a local minimum is observed for phonons with a longer wavelengths (smaller q), and the position of the minimum shifts to the right with increasing A_{DB}. This local minimum can be attributed to the resonance of the phonon wavelength with the DB width, which decreases with increase in A_{DB}.

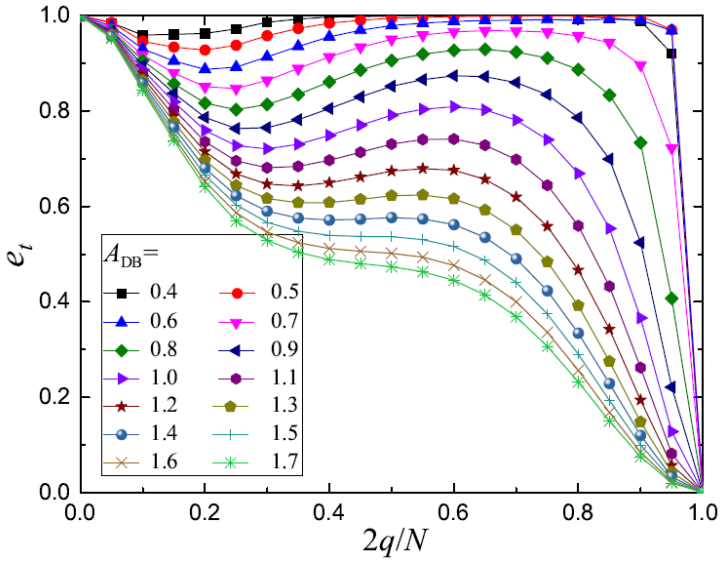

Fig. 3. The transmission coefficient defined by (10) as the function of the normalized phonon wavenumber for different DB amplitudes A_{DB} from 0.4 to 1.7, as indicated for each curve in the inset.

The mean integral transmission coefficient,

$$I_t = \frac{2}{N} \int_0^{N/2} \varepsilon_t dq , \tag{11}$$

is plotted in Fig. 4 as the function of the DB amplitude by dots connected by the blue line. We note once again that, for $A_{DB} < 0.5$, the DB has practically no effect on the phonon flux, since I_t is close to unity. For $A_{DB} > 0.5$ the DBs start to noticeably reflect the short-wavelength phonons and I_t starts to decrease with increasing A_{DB}.

Phonon energy density is

$$E = \frac{1}{2} e^2 \omega_q^2 . \tag{12}$$

In thermal equilibrium, by definition, all phonon modes have equal energy density. A phonon carries energy with the group velocity defined by (7). All phonons moving in positive direction ($q>0$) carry energy

$$W_0\int_0^{N/2} E\upsilon_g dq = 2E\sqrt{\frac{k}{m}}\,. \tag{13}$$

If a DB is in the chain, only a part of the energy will pass through it, which can be calculated as

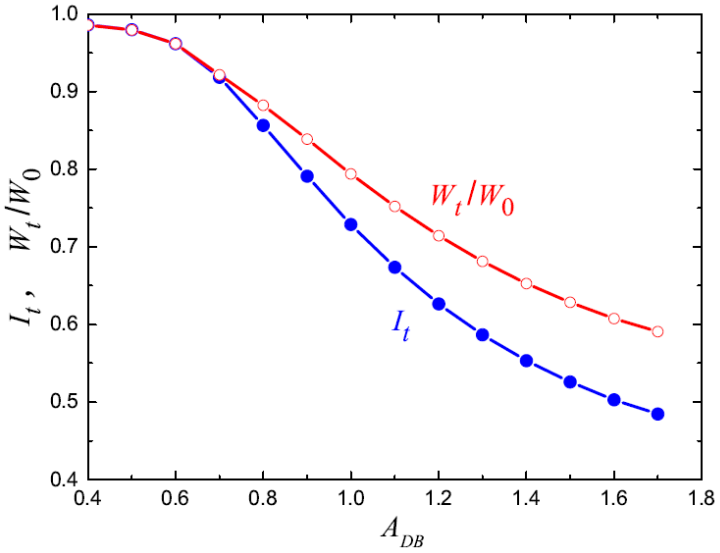

Fig. 4. I_t (filled dots) and W_t/W_0 (open symbols) as the functions of DB amplitude.

$$W_t = \int_0^{N/2} e_t(q)\,E\upsilon_g dq \tag{14}$$

and this energy depends on the DB amplitude because $e_t(q)$ depends on it.

We estimate W_t numerically taking $e_t(q)$ from Fig. 3 for various DB amplitudes and present the ratio W_t/W_0 , in Fig. 4 by open symbols connected with the red line. This curve lies above the $I_t(A_{DB})$, curve, since it characterizes the integral effect of DBs on energy transfer by phonons, taking into account the fact that short-wavelength phonons have a smaller group velocity; for instance, at $A_{DB}=1.7$ one has $I_t=0.48$ and $W_t/W_0=0.59$.

5. Conclusions

In the present study, the scattering of small-amplitude phonons by DBs was analyzed numerically in the β-Fermi–Pasta–Ulam–Tsingou (β-FPUT) chain with the hard type anharmonicity ($\beta>0$). As in the case of a hard type anharmonicity chain with an on-site potential, studied in [53], the DBs in the β-FPUT chain mainly reflect short-wavelength phonons, being practically transparent for long-wavelength phonons. This contrasts with the soft type anharmonicity chain with on-site potential, for which the opposite trend was observed [53].

The DB scatters short-wavelength phonons only if its amplitude is higher than the threshold value, in the chain under consideration scattering takes place at $A_{DB}>0.5$. This fact explains the relatively

sharp transition from ballistic to normal heat conductivity with increasing temperature in the nonlinear chain (see [42]). At low temperatures, only small-amplitude DBs are excited; they weakly interact with phonons and do not change the character of ballistic thermal conductivity. At sufficiently high temperature, large-amplitude DBs are excited, which change the thermal conductivity to normal characteristics, acting as defects scattering phonons.

In the β-FPUT chain, the effect of the DBs on thermal conductivity should be relatively small, since DBs mainly scatter short-wavelength phonons, which have a low group velocity and, therefore, make an insignificant contribution to thermal conductivity.

Our results confirm the conclusion that thermally populated DBs can reduce thermal conductivity at high temperatures due to phonons scattering [42]. In subsequent works, the case of not very small phonon amplitudes will be considered, when new interesting effects can be observed, such as emission of energy by a discrete breather, acceleration of a mobile DB by phonons, and others. It would also be interesting to consider if strong anharmonicities in this model could induce properties typical of liquids, such as linear in frequency vibrational density of states [56], and/or anomalous glassy properties, such as an anomaly in the Boson Peak at low energies [57].

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