PACS 63.20.Pw, 44.10.+i

Discrete breathers: possible effects on heat transport

Daxing Xiong†, Jun Zhang

†phyxiongdx@fzu.edu.cn

Department of physics, Fuzhou University, Fuzhou, 350108, Fujian, China

Discrete breathers (DBs), also known as intrinsic localized modes, are spatially localized nonlinear vibrational modes in defected-free anharmonic lattices and expected to affect energy transfer process. However, whether DBs can contribute to thermal transport at finite temperature is still not very clear. In the present work, we briefly describe our recent results on the possible effects of DBs on heat transport. By employing two one-dimensional (1D) anharmonic lattice models with different phonon dispersions, we provide some numerical evidences to demonstrate that given the peculiar phonon dispersions along with nonlinearity, two kinds of DBs, i.e., the intra-band and extra-band ones, can exist in 1D lattices at finite temperature and thus contribute to thermal transport in different ways, i.e., the intra-band DBs can be scattering with phonons; while the extra-band DBs mainly localize the system energies, thus both tend to limit the heat transport in the thermodynamic limit. Our results here suggest that different peculiar phonon dispersions along with nonlinearity can enable us to excite different types of DBs, which then affect the heat transport process in different ways. These results may provide useful information for establishing the connection between the macroscopic heat transport process and the underlying DBs dynamics in general 1D nonlinear systems with various phonon dispersions.

Keywords: discrete breathers, heat transport.

1. Introduction

In the past decade of the last century, discrete breathers (DBs), also known as intrinsic localized modes, had been a hot topic of nonlinear science [1-3]. Huge numbers of theoretical studies had devoted to confirm the existence and stability of DBs [4-6]. Recently there are also many experimental investigations on observation of DBs in real crystals [7-11]. Nevertheless, most of the existing theoretical works were only limited to the case of the focused systems with zero temperature, while only quite few understanding about the existence of DBs at finite temperature have been reported [12, 13]. Given DBs in thermal equilibrium, it is thus tempting to ask whether DBs can contribute to thermal transport in crystals.

In this work we briefly introduce our recent results [14-16] on the possible roles of DBs in thermal transport. We will mainly employ two one-dimensional (1D) lattice models to describe our viewpoints. Thus, the rest of this article is organized as follows: In Sec. 2 the focused models are presented and their peculiar phonon dispersions are emphasized. With their phonon dispersions in mind, Sec. 3 provides the results of DBs properties at finite temperature. In Sec. 4 we then try to relate the DBs properties to heat transport behavior. Finally, the last section summarizes our conclusion.

2. Models

To illustrate our idea that DBs can contribute to heat transport, we consider the following two 1D lattice models, i.e., (i) Model I: the chain with both nearest-neighbor (NN) and next-nearest-neighbor (NNN) couplings [14, 16], and (ii) Model II: the chain with alternating interactions [15], whose dimensionless Hamiltonian can be represented by

$$H = \sum_{m=1}^{L} \frac{p_m^2}{2} + V\left(x_{m+1} - x_m\right) + \gamma V\left(x_{m+2} - x_m\right); \qquad (1)$$

$$H = \sum_{m=1}^{L/2} \frac{p_{2m-1}^2}{2} + \frac{p_{2m}^2}{2} + k_1 V\left(x_{2m} - x_{2m-1}\right) + k_2 V\left(x_{2m+1} - x_{2m}\right), \qquad (2)$$

respectively, where p_m denotes the momentum and x_m denotes the displacement from equilibrium position for the m-th particle. To include the nonlinearity, both potentials take the Fermi-Pasta-Ulam-β form as $V(m) = m^2/2 + m^4/4$ ($\beta = 1$). In Model I, the parameter γ denotes the comparative strength of the NNN coupling to the NN coupling; while in Model II, k_1 and k_2 ($k_1 \le k_2$) represent the adjacent interactions coupling strengths. For the latter model, usually we can fix $k_1 + k_2 = 2$ and define $\gamma = k_1/k_2$ ($\gamma \le 1$) as a controlled parameter.

Given the Hamiltonian, then both models phonon dispersions can be readily obtained under linear harmonic approximation:

$$\omega = 2\sqrt{\sin^2\left(\frac{q}{2}\right) + \gamma \sin^2\left(q\right)}; \qquad (3)$$

$$\omega^{\pm} = \left[k_1 + k_2 \pm \sqrt{k_1^{\,2} + k_2^{\,2} + 2k_1k_2\cos\left(2q\right)}\right]^{\frac{1}{2}}, \qquad (4)$$

with q the wave number and ω the coorresponding frequency [in Eq. (4) ω^+ (ω^-) denotes the case of optical (acoustic) phonons].

In Fig. 1 we plot ω vs q according to Eqs. (3) and (4), from which both models peculiar dispersions can be clearly seen,

i.e., the dispersions are strongly depenent on the controlled parameter γ. In particular, there is a turning point of $\gamma = 0.25$ for Model I, where the values of phase velocity of phonons (defined by $v = d\omega/dq$) emerge most at $v = 0$ near the Brillouin zone ($q \to \pm\pi$); while in the Model II, as long as $\gamma \neq 0$, there is a gap between the acoustic and optical phonons. We expect that such key unusual propeties of dispersions along with nonlinearity may support the exsitence of DBs and thus affect heat transport behavior.

3. DBs properties

In view of both γ dependence of dispersions, in this section we will mainly focus on how the DBs properties would depend on γ at a given model temperature $T = 2.5$. To obtain DBs at the focused temperature, usually we can employ the following numerical method [17]: A chain of $L = 2000$ particles is initially thermalized with heat baths [18]; then the heat baths are removed, and the absorbing boundary conditions are imposed [19]. If DBs can exist, after a long enough time for absorption, leading all the mobile excitations, such as phonons and solitary waves absent, DBs then would show up in the internal segment of the chain.

Following this way we then can idendify DBs at a finite temperature. As some examples, we plot some snapshots of signgle DB's profiles for both models in Fig. 2 and Fig. 3. As can be seen, both models signgle DB's profiles also show γ dependence: (i) for Model I, we can clearly identify a transtion from Page mode [$\gamma < 0.25$, see Fig. 2(a)] [20] to Sievers-Takeno mode [$\gamma > 0.25$, see Fig. 2(c)] [20], among which at $\gamma = 0.25$ we aslo see the envelope DBs with long tails [see Fig. 2(b)]; while for Model II, there is a transition from Page mode to moving DBs [see Fig. 3(d)], especially under certain γ values about $\gamma = 0.34$, we can also find a profile which looks like the case of two kinks of solitons trapped by two DBs [see Fig. 3(c)]. All of the reported results here clearly indicate that the dynamics of DBs in both models are rich after taking the peculiar phonon dispersions into account.

4. Relating DBs to heat transport

Now let us see how the above DBs γ-dependent dynamics may be related to heat transport. For this purpose, we first present our results on γ-dependent heat conduction behavior (see Fig. 4). Our results will mainly focus on how the length divergence exponent α [21] of heat conductivity depends on the controlled parameter γ. For each γ and system size, we employ the the reverse nonequilibrium molecular dynamics (RNEMD) simulation method [22] to produce the heat flux and then obtain the heat conductivity, finally get the divergence exponent α (see [14] for simulation details).

As can be seen from Fig. 4, both systems heat conduction behavior show intriguing nonmonotonic γ dependence with a turning point of $\gamma_{tr} = 0.25$, suggesting that α might not have its universality in heat transport of 1D systems as conjectured previously in the literatures [21]. Interestingly, this turning point of $\gamma_{tr} = 0.25$ appears to be related to the turning point of phonon dispersions [see Fig. 1(a) for example] and DBs properties (see Fig. 2).

In order to further verify this relation, we then carefully examine the power spectra $P(\omega)$ of the residual thermal fluctuaions for both models, which can be regarded as the spectra of emerging DBs along the chain at the focused temperature. To measure $P(\omega)$, for each γ, we take the same strategy as to obtain DBs but with a short lattice of 200

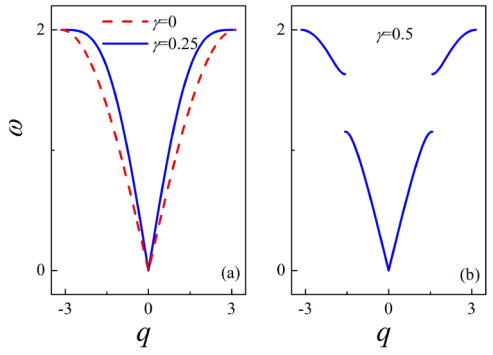

Fig. 1. The phonon dispersions for Model I (a) and Model II (b), respectively.

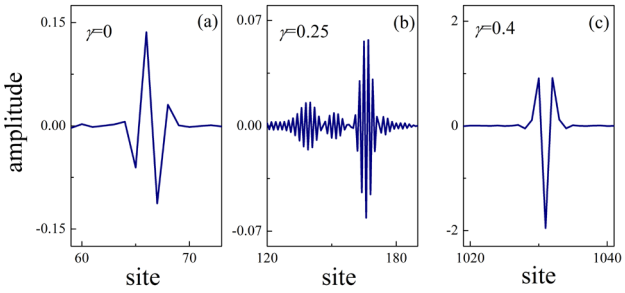

Fig. 2. The DBs profiles after long time absorption for Model I with $\gamma = 0$; $\gamma = 0.25$ and $\gamma = 0.4$, respectively.

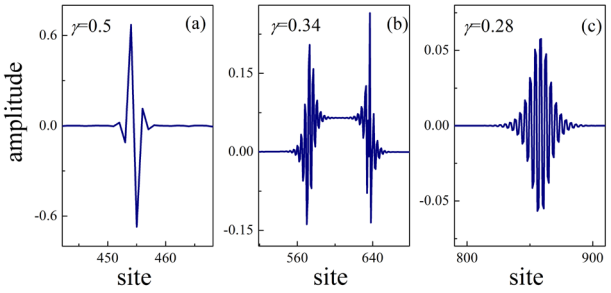

Fig. 3. The DBs profiles after long time absorption for Model II with $\gamma = 0.5$; $\gamma = 0.34$ and $\gamma = 0.28$, respectively.

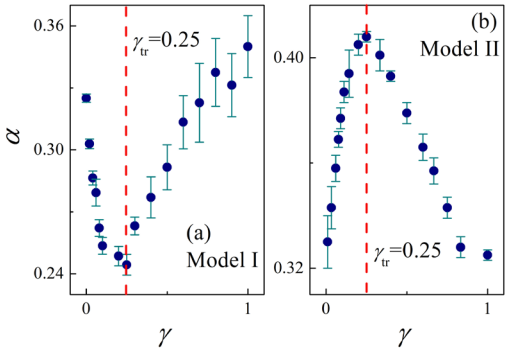

Fig. 4. The divergence exponent α of heat conduction depends on the controlled parameter γ for Model I (a) and Model II (b), respectively.

particles instead for facilitating the computation. After all of the DBs are emerging we then anlysize their $P(\omega)$. The final results are obtained by taking 100 instances of simulation with different initial conditions for the average.

The main results are shown in Fig. 5 and Fig. 6, from which, though we can clearly identify that in both models there is a γ-dependent manner of DBs power spectra information; the details are different: (i) in Model I, the DB frequencies are mainly outside the linear phonon band [$\omega > 2$, see Fig. 5 (a) and (c)], however, at $\gamma_{tr} = 0.25$ a significant portion of the DB frequencies appearing inside the linear phonon band can be seen [$\omega < 2$, see the inset of Fig. 5 (b)]; (ii) for Model II, as γ decreases from 1 to 0, we can find a transition from optical DBs [with frequencies above the optical phonons frequency, see Fig. 6(a)-(b)] to gap DBs [with frequencies lying in the gap between acoustic and optical phonons, see Fig. 6(e)]. Interestingly, there are two kinds of gap DBs with the frequencies slightly above the acoustic phonons, or slightly below the optical phonons. In particular, $\gamma = 0.25$ is a turning point, at which the two kinds of gap DBs have close spectrum strength.

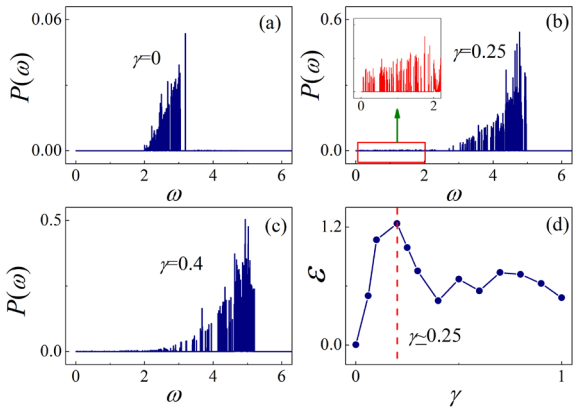

Fig. 5. The power spectrum of DBs in the case of Model I for (a) $\gamma = 0$; (b) $\gamma = 0.25$ and (c) $\gamma = 0.4$, respectively. The inset in (b) is a zoom for the boxed intraband components ($\omega \leq 2$). (d) The energy portion ε of the DBs within the phonon band. The vertical dashed line indicates the turning point of $\gamma_{tr} \approx 0.25$.

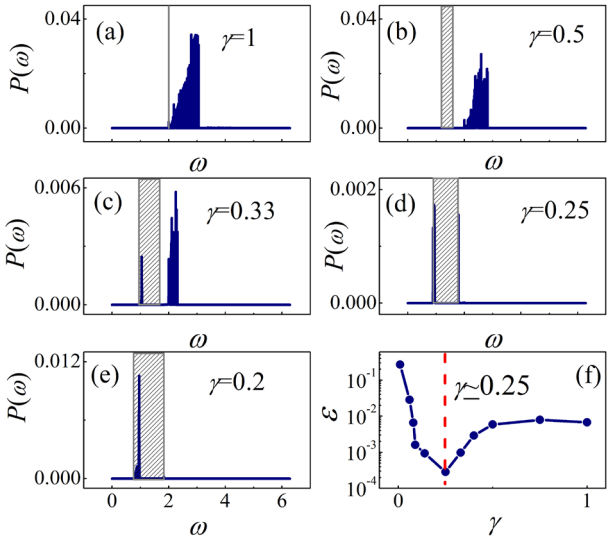

Fig. 6. The power spectrum of DBs in the case of Model II for (a) $\gamma = 1$; (b) $\gamma = 0.5$; (c) $\gamma = 0.33$; (d) $\gamma = 0.25$ and (e) $\gamma = 0.2$, respectively. The shaded area indicates the gap of the linear spectra between the acoustic and optical branches for each γ (f) The energy ratio ε of the DBs to the intital energy without absorption. The vertical dashed line indicates the turning point of $\gamma_{tr} \approx 0.25$.

Given the above DBs frequency details, it is then natural to conjecture that, DBs can be mainly classified into two categories, i.e., the extra-band ones and the intra-band ones, according to whether their frequencies are within the linear phonons band. The effects of the extra-band DBs may mainly be localizing the system energies; however, the intraband DBs can be scattering with phonons since they have frequencies lying in the phonons band. With these two different mechanisms in mind, we then further define

$$\text{(i)} \qquad \varepsilon = \int_0^2 P(\omega)\mathrm{d}\omega \Big/ \int_0^\infty P(\omega)\mathrm{d}\omega,$$

the ratio of the energy of the collective modes within the linear phonon band to the total energy of DBs, to measure the relative proportion of intra-band DBs for Model I; and

$$\text{(ii)} \qquad \varepsilon = \int_0^\infty P(\omega)\mathrm{d}\omega \Big/ \int_0^\infty P_0(\omega)\mathrm{d}\omega$$

[$P_0(\omega)$ and $P(\omega)$ are the power spectra of the initial thermal fluctuations and that after the absorption], the ratio of the residual energy after the absorption to the initial energy, to measure the localization of energy induced by DBs for Model II. Our results of $\varepsilon(\gamma)$ are presented in Fig. 5(d) and Fig. 6(f). From the Figs. 5-6 and compared with the previous results of Fig. 4, we can clearly recognize a positive correlation between $\varepsilon(\gamma)$ and $\alpha(\gamma)$, suggesting that the DBs properties should be related to heat transport. We thus suggest the following underlying pictures for the relationship: (i) in Model I, the effects are mainly caused by intra-band DBs, then suppose the scattering between phonons and the intra-band DBs can be described by $\varepsilon(\gamma)$, so a stronger (weaker) scattering will finally limit (facilitate) the heat transport in the thermodynamic limit, which supports the behavior of $\alpha(\gamma)$; (ii) for Model II, there are only extra-band DBs, then it can be expected that a smaller (larger) ε will lead to less (more) energy localization, finally facilitate (limit) heat transport in the thermodynamical limit, hence supporting the results of $\alpha(\gamma)$. It is worth noting that from Figs. 4-6, the heat transport and DBs simulation results are indeed in accod with our explanations, thus supporting that DBs should have their effects on heat transport in crystals.

5. Conclusions

In summary, we have briefly described our recent results on how DBs are related to heat transport in crystals. We have numerically demonstrated that DBs can exist at finite temperature in the two focused 1D anharmonic lattices with very peculiar phonon dispersions. Induced by the different dispersions along with nonlinearity, we are able to identify two different types of DBs in each system, i.e., the intra-band and extra-band ones; and we conjecture that their roles in heat transport may be different, i.e., the intra-band DBs can be scattering with phonons, while the extra-band DBs will mainly localize energy. With this conjecture we have showed that the quite unusual heat transport behaviors observed in

these systems can be well understood. The reported results here apparently provide evidences that DBs can contribute to heat transport in crystals.

Acknowledgements. This work was supported by National Science Foundation of china, mainly under the following two grants: No. 11205032 and No. 11575046. The authors wish to acknowledge Profs. Hong Zhao; Jiao Wang, and Yong Zhang, for their significant contributions to this work.

References

1. S. Flach, A. V. Gorbach. Phys. Rep. **467**, 1 (2008).
2. S. Flach, C. R. Willis. Phys. Rep. **295**, 181 (1998).
3. S. V. Dmitriev, A. P. Chetverikov, M. G. Velarde. Phys. Status. Solidi B **252**, 1682 (2015).
4. A. J. Sievers, S. Takeno. Phys. Rev. Lett. **61**, 970 (1988).
5. J. B. Page. Phys. Rev. B **41**, 7835 (1990).
6. R. S. MacKay, S. Aubry. Nonlinearity **7**, 1623 (1994).
7. N. K. Voulgarakis, G. Kalosakas, A. R. Bishop, G. P. Tsironis. Phys. Rev. B **64**, 020301 (R) (2001).
8. G. Kalosakas, A. R. Bishop, A. P. Shreve. Phys. Rev. B **66**, 094303 (2002).
9. M. E. Manley, M. Yethiraj, H. Sinn, H. M. Volz, A. Alatas, J. C. Lashley, W. L. Hults, G. H. Lander, J. L. Smith. Phys. Rev. Lett. **96**, 125501 (2006).
10. M. E. Manley, J. R. Jeffries, H. Lee, N. P. Butch, A. Zabalegui, D. L. Abernathy. Phys. Rev. B **89**, 224106 (2014).
11. B. I. Swanson, J. A. Brozik, S. P. Love, G. F. Strouse, A. P. Shreve, A. R. Bishop, W. Z. Wang, M. I. Salkola. Phys. Rev. Lett. **82**, 3288 (1999).
12. L. Z. Khadeeva, S. V. Dmitriev, and Yu. S. Kivshar. JETP Lett. **94**, 539 (2011).
13. M. V. Ivanchenko, O. I. Kanakov, V. D. Shalfeev, S. Flach. Physica D **198**, 120 (2004).
14. D. Xiong, J. Wang, Y. Zhang, H. Zhao. Phys. Rev. E **85**, 020102 (R) (2012).
15. D. Xiong, Y. Zhang, H. Zhao. Phys. Rev. E **88**, 052128 (2013).
16. D. Xiong, Y. Zhang, H. Zhao. Phys. Rev. E **90**, 022117 (2014).
17. G. P. Tsironis, A. R. Bishop, A. V. Savin, A. V. Zolotaryuk. Phys. Rev. E **60**, 6610 (1999).
18. S. Nose. J. Chem. Phys. **81**, 511 (1984); W. G. Hoover. Phys. Rev. A **31**, 1695 (1985).
19. G. P. Tsironis, S. Aubry. Phys. Rev. Lett. **77**, 5225 (1996).
20. S. Flach, A. Gorbach. Chaos **15**, 015112 (2005).
21. It has been realized that in 1D momentum-conserving systems, usually the heat conductivity follows a power law with the system size L as L^{α}; see the following reviews: S. Lepri, R. Livi, A. Politi. Phys. Rep. **377**, 1 (2003); A. Dhar. Adv. Phys. **57**, 457 (2008).
22. F. Müller-Plathe. J. Chem. Phys. **106**, 6082 (1997) .