PHYSICAL REVIEW E **85**, 020102(R) (2012)

# Nonuniversal heat conduction of one-dimensional lattices

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(Received 24 August 2011; published 1 February 2012)

For one-dimensional nonlinear lattices with momentum conserving interparticle interactions, intensive studies have suggested that the heat conductivity $\kappa$ diverges with the system size $L$ as $\kappa \sim L^{\alpha}$ and the value of $\alpha$ is universal. But in the Fermi-Pasta-Ulam-$\beta$ lattices with nearest-neighbor (NN) and next-nearest-neighbor (NNN) coupling, we find that $\alpha$ strongly depends on $\gamma$, the ratio of the NNN coupling to the NN coupling. The correlation between the $\gamma$-dependent heat conduction behavior and the in-band discrete breathers is also analyzed.

DOI: 10.1103/PhysRevE.85.020102 PACS number(s): 05.60.−k, 44.10.+i, 63.20.Pw, 63.20.Ry

In the studies of nonelectronic heat conduction, it is an important step of progress to realize that the heat conductivity $\kappa$ diverges with the system size $L$ as $\kappa \sim L^{\alpha}$ in one-dimensional nonlinear chains with momentum conserving interactions [1,2]. The value of the exponent $\alpha$ is believed to be constant and universal [3], though there are many debates on what value(s) it takes. (For example, if there exists one universal class with $\alpha = \frac{1}{3}$ [4,5] or two with $\alpha = \frac{1}{3}$ and $\alpha = \frac{2}{5}$ [6–8] is still controversial.) The universality of $\alpha$ roots in the theory first proposed by Peierls [9], where the essence of the nonelectronic heat conduction is modeled as a weakly interacting phonon gas at *low* temperatures. Based on this model, a universal heat conduction law constrained only by the dimensionality of a system, regardless of the details of its microscopic dynamics, is thereby expected.

On the other hand, at *high* temperatures nonlinear excitations such as traveling solitary waves [10] and discrete breathers (DBs) [11] are ubiquitous in nonlinear lattices; hence the interactions between phonons and nonlinear excitations should be studied and taken into account when their effects are considerable. As nonlinear excitations involve microscopic dynamical details, whether a universal heat conduction law still exists certainly deserves careful investigations. In this respect quite a few studies have been reported. Early work by our group showed that traveling solitary waves may play an important role in heat conduction of the Fermi-Pasta-Ulam-$\beta$ (FPU-$\beta$) chains [12,13], but this was argued against by some authors [14,15]. In addition, DBs have also been proposed as a phonon scattering mechanism [16] for the normal heat conduction (i.e., $\kappa$ converges in the thermodynamical limit) numerically observed in the harmonic chains with on-site potentials [17] and in the rotator chains [18]. However, in spite of these studies, at present whether and, if yes, how the nonlinear excitations would affect the heat transport in low-dimensional momentum conserving systems is still an open question.

In this Rapid Communication we present strong evidence of the nonuniversal heat conduction behavior. Specifically, we perform numerical analysis to investigate the heat conduction in one-dimensional FPU-$\beta$ chains with both the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) coupling. Our results show that the value of $\alpha$ varies *continuously* with the ratio of the NNN coupling to the NN coupling, suggesting the system does not belong to any universality class characterized by a constant $\alpha$. Moreover, we find $\alpha$ is correlated to the overlap of the phonons' spectra and the DBs' spectra, which is consistent with the assumption that DBs may provide a new phonon scattering mechanism and thus have implications on the heat conduction behavior of the system [16].

Our model is a chain of $N$ identical particles with both the NN and NNN interactions [19] whose Hamiltonian is

$$H = \sum_i \left[ \frac{p_i^2}{2\mu} + V(x_{i+1} - x_i) + \gamma V(x_{i+2} - x_i) \right]. \quad (1)$$

Here $x_i$ is the displacement of the $i$th particle from its equilibrium position and $p_i$ is its momentum. The potential is of the FPU-$\beta$ type; i.e., $V(x) = \frac{1}{2}x^2 + \frac{1}{4}x^4$. Both the mass $\mu$ and the lattice constant are set to be unity. The parameter $\gamma$ is tunable; it specifies the comparative strength of the NNN coupling. $\gamma = 0$ corresponds to the conventional FPU-$\beta$ system.

We employ the reverse nonequilibrium molecular dynamics simulation method (RNEMD) [20] to build the nonequilibrium stationary state across the system. Compared with the usual method that brings the two ends of system in contact with two heat baths at different temperatures, it is advantageous in suppressing the boundary effects and therefore leads to a faster convergence to the stationary state. Meanwhile it keeps the total energy and momentum of the system unchanged. Let us consider a chain of $N$ particles. Following the prescription of RNEMD [20] the periodic boundary condition is imposed to make the chain form a circle, and then the circle is divided into $M$ ($M$ being even) slabs of equal size, each containing $n = \frac{N}{M}$ particles. Next, two opposite slabs chosen arbitrarily are set to be the cold and the hot slab, respectively. For the sake of convenience, we give each slab a serial number and assign the cold slab to be slab 1 and, accordingly, the hot one to be slab $\frac{M}{2} + 1$. The key idea of RNEMD is that, as the system evolves, the momentum of the hottest particle in the cold slab is *artificially* interchanged with that of the coldest particle in the hot slab at a frequency denoted by $f_{\mathrm{exc}}$. This procedure forces a redistribution of kinetic energy $\Delta E = \sum \frac{1}{2\mu}(p_h^2 - p_c^2)$ during time $t$ between the cold and the hot slab. (Here the subscripts $h$ and $c$ refer to the hottest and coldest particles

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whose momenta are exchanged, and the sum runs over all exchange events in time $t$.) As a consequence, the relaxation of $\Delta E$ will drive the flow of two heat fluxes from the hot slab to the cold slab along the two "semicircular" sides (with an effective length of $L = \frac{N}{2} - n$) bridging them. In the stationary state eventually reached, we measure the heat flux across each side $\langle J \rangle \equiv \lim_{t\to\infty} \frac{\Delta E}{2t}$ and the temperature profile of the system, represented by the time averaged kinetic temperature of every slab, denoted by $\langle T_k \rangle$ for slab $k$. The instantaneous local kinetic temperature $T_k \equiv \frac{1}{n\mu k_B} \sum_{i=n(k-1)+1}^{nk} p_i^2$, where $k_B$ is the Boltzmann constant (set to be unity) and the sum runs over all $n$ particles in slab $k$. The heat conductivity can then be obtained, and it reads $\kappa = -\langle J \rangle / \nabla T$, with the temperature gradient $\nabla T$ being evaluated over the slabs between the cold and the hot one.

We start our simulations with a fully thermalized chain at temperature $T = 2.5$. The velocity-Verlet algorithm [21] with a time step of 0.01 is used to evolve the system, and $M = 80$ and $f_{\rm exc} = 0.1$ are adopted for the RNEMD. For each system size a transient stage of time $10^6$, which has been verified to be long enough for reaching the stationary state, is discarded; then the next evolution of time $10^7$ is performed for the time average. We have verified that our results do not significantly depend on the particular simulation details taken here.

Before presenting our main results, it is interesting to make a quick comparison between our simulations and those by different methods. For $\gamma = 0$, i.e., the conventional FPU-$\beta$ system, Fig. 1(a) shows our result of the temperature profile for $L = 2496$. It can be seen that a constant temperature gradient is well established between the cold and the hot slabs. In addition, for larger system sizes the temperature profiles (not shown) have been checked to be the same upon a rescaling. Figure 1(c) shows the dependence of $\kappa$ on the effective system size $L$; it suggests that $\kappa$ diverges as $L \sim L^\alpha$ with $\alpha = 0.325 \pm 0.002$, which we emphasize to be very close to the predicted value $\frac{1}{3}$ by the hydrodynamic theory [4] and the result of a recent careful numerical study [5]. For $\gamma = 1$ we have obtained similar results [see Figs. 1(b) and 1(d)], but the best fitting

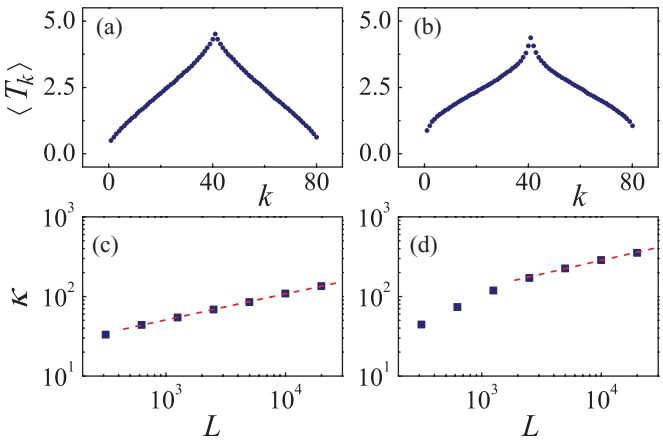


FIG. 1. (Color online) The temperature profile for (a) $\gamma = 0$ and (b) $\gamma = 1$ with the effective system size $L = 2496$. The heat conductivity $\kappa$ vs $L$ for (c) $\gamma = 0$ and (d) $\gamma = 1$. The dashed lines are for the best fitting of $\kappa \sim L^\alpha$, suggesting $\alpha = 0.325 \pm 0.002$ for $\gamma = 0$ (c) and $\alpha = 0.35 \pm 0.02$ for $\gamma = 1$ (d).

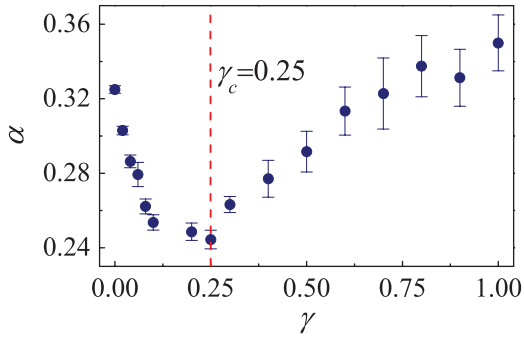


FIG. 2. (Color online) The dependence of $\alpha$ on parameter $\gamma$. The vertical dashed line indicates $\gamma_c = 0.25$. Error bars give the standard error for evaluating $\alpha$ by linearly fitting $\ln \kappa$ vs $\ln L$.

performed over $2496 \leqslant L \leqslant 19968$ suggests $\alpha = 0.35 \pm 0.02$ instead [see Fig. 1(d)]. Note that our $\alpha$ value for $\gamma = 1$ is remarkably different from that given in Ref. [19], where $\alpha$ was evaluated over much shorter system sizes ($L < 2000$) so that it fails to correctly capture the divergence of $\kappa$ in the thermodynamical limit.

Figure 2 presents our main result, where the dependence of the divergence exponent $\alpha$ on the parameter $\gamma$ is investigated. It can be seen that, as $\gamma$ changes from 0 to 1, $\alpha$ decreases and reaches its minimum $\alpha_{\rm min} \approx 0.25$ at $\gamma \approx \gamma_c = 0.25$ and then increases up to about 0.35 at $\gamma = 1$ with a trend of saturation [22]. The fact that $\alpha$ changes continuously is in clear contrast to the existence of a general $\alpha$ value(s) independent of the dynamics.

As phonons are the heat energy carriers in our system, the fact that $\alpha$ takes its minimum at $\gamma_c$ implies that the NNN coupling may enhance the phonon scattering for $\gamma$ being close to $\gamma_c$. To probe the underlying scattering mechanism, the phonon dispersion relation turns out to be very suggestive. Keeping only the harmonic terms in both the NN and NNN interactions, the dispersion relation reads $\omega_q = 2[\sin^2 \frac{q}{2} + \gamma \sin^2 q]^{\frac{1}{2}}$, where $q$ is the wave number and $\omega_q$ is the corresponding frequency. Interestingly, $\gamma_c$ is a transition value for the phonon dispersion relation as well (see Fig. 3): For $\gamma \leqslant \gamma_c$ the maximum frequency corresponds to the boundary of the Brillouin zone at $q = \pi$, which is $\omega_\pi = 2$, but for

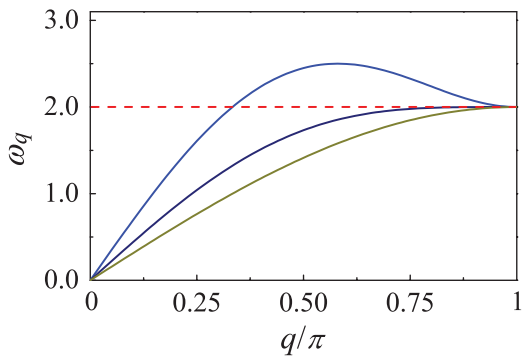


FIG. 3. (Color online) Phonon dispersion relation for the FPU-$\beta$ system with the NNN interactions. From bottom to top, the curves correspond to $\gamma = 0$, 0.25, and 1, respectively. The horizontal dashed line indicates $\omega_\pi = 2$.

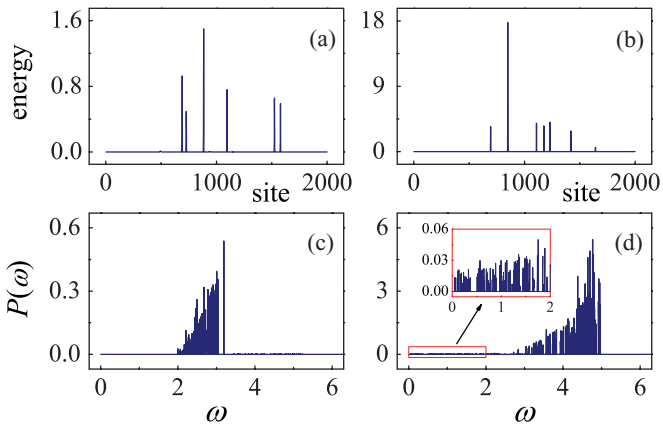


FIG. 4. (Color online) (a) and (c) Snapshots of the energy distribution and the power spectrum of the residual thermal fluctuations for $\gamma = 0$. (b) and (d) The corresponding results for $\gamma = 0.25$. The power spectrum in (c) and (d) takes an arbitrary unit. The inset in (d) is a zoom for the boxed in-band components.

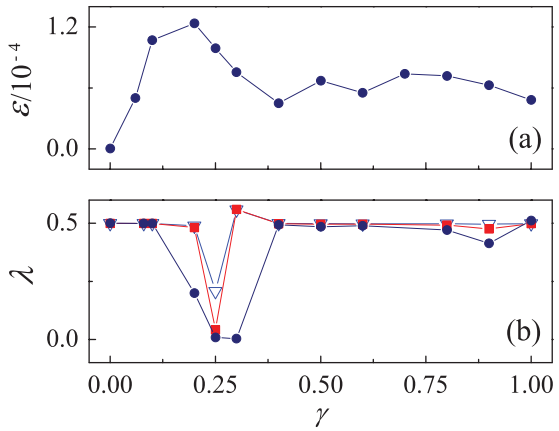


FIG. 5. (Color online) (a) The energy portion of the residual thermal fluctuations within the phonon band. (b) $\lambda$ vs $\gamma$ for $e(0) =$ 0.005 (triangles), 0.045 (squares), and 0.18 (dots).

$\gamma > \gamma_c$, it grows larger than $\omega_\pi$, and the corresponding $q$ value decreases away from $q = \pi$. For $\gamma = \gamma_c$ the group velocity $v_g = d\omega_q/dq$ is close to zero in a wider $q$ domain close to the Brillouin zone boundary. This property favors the formation of DBs in the presence of the nonlinearities [23], which will be shown later [see Fig. 5(b)].

It has been known that the temperature activated DBs may be crucial for the energy transport and other dynamical processes following the work by Peyrard [24]. Interesting examples include the melting transitions in solids and folding in polypeptide chains [25]. To study if DBs may have any effects on heat conduction in our system, the first step is to check if DBs exist at the focused temperature $T = 2.5$. We apply the method given in Ref. [17]: A chain of $N = 2000$ particles is initially thermalized at temperature $T = 2.5$; then the heat baths are removed, and the absorbing boundary conditions are imposed [26]. If DBs exist, after all the mobile excitations such as phonons and solitary waves are absorbed, they may show up in the internal segment of the chain. In this way the DBs have been identified. As an example, the snapshot of the energy profile after a long time ($8 \times 10^5$) absorbtion is presented in Figs. 4(a) and 4(b) for $\gamma = 0$ and $\gamma = \gamma_c$, respectively. In both plots the DBs can be well recognized. We have verified that this is also the case for other $\gamma$ values in [0,1].

Now we study how the properties of the DBs may depend on parameter $\gamma$. We calculate the power spectra $P(\omega)$ of the residual thermal fluctuations after long time absorbtion; i.e., the set of all DBs emerges eventually. To facilitate the computation short chains of size $N = 200$ are considered. The results for $\gamma = 0$ and $\gamma = \gamma_c$ are plotted in Figs. 4(c) and Fig. 4(d) for a comparison, which shows that for $\gamma = 0$ the DB frequencies are outside the linear phonon band of $0 \leqslant \omega \leqslant \omega_\pi$, in agreement with the classical DB theory [27]. However, in clear contrast, for $\gamma = \gamma_c$ a significant portion of the DB frequencies appear inside the linear phonon band, suggesting the existence of the in-band DBs [28–30]. In the inset in Fig. 4(d) the collective modes in the linear phonon band can be clearly recognized.

Based on these results, a natural *conjecture* is that it is the in-band DBs that have interactions with phonons. Given this, the lack of the in-band DBs in the former case of $\gamma = 0$ implies they have no effects on heat conduction; hence the Peierls phonon gas model is still valid for understanding the general $\alpha = \frac{1}{3}$ behavior observed. But for $\gamma = \gamma_c$, as the in-band DBs randomly distribute along the lattice, they introduce an inherent disorder [27] and may serve as random scatters to the phonons. This may explain why $\alpha$ becomes smaller.

If this conjecture is correct, combining the results given in Fig. 2, we may expect that as $\gamma$ is increased, the interactions between the in-band DBs and the phonons would become stronger and stronger (weaker and weaker) for $0 \leqslant \gamma \leqslant \gamma_c$ ($\gamma_c < \gamma \leqslant 1$). As a measure of the interaction intensity between the in-band DBs and the phonons, we assume $\varepsilon = \int_0^{\omega_\pi} P(\omega)d\omega / \int_0^{\infty} P(\omega)d\omega$, the ratio of the energy of the collective modes within the linear phonon band to the total energy of the residual thermal fluctuations. For several different $\gamma$ values we have calculated the corresponding power spectrum in the same way as in Figs. 4(c) and 4(d) and evaluated $\varepsilon$ and summarized the results in Fig. 5(a). A positive correlation between $\varepsilon$ and $\alpha$ (see Fig. 2) can be clearly recognized. [Note that in Fig. 5(a) the maximum of $\varepsilon$ does not correspond to $\gamma_c$ exactly but rather a slightly smaller $\gamma$ value; this discrepancy may be a result of the big statistical errors in the evaluated power spectra of the residual thermal fluctuations where short chains of $N = 200$ have to be used because of computation cost.]

Now let us turn to the question why the DB-phonon interactions could be the strongest at $\gamma = \gamma_c$. Our study in the following suggests the DB concentration is the highest at $\gamma = \gamma_c$, which we conjecture to be the reason. The concentration of DBs in an equilibrium state is approximately $e^{-\frac{e_{\rm sh}}{k_B T}}$, where $e_{\rm sh}$ is the energy threshold for creating the DBs [27]. It implies that if DB concentration is the highest at $\gamma = \gamma_c$, then the corresponding $e_{\rm sh}$ should be the smallest. To check if this is the case we consider an energy relaxation process on a chain of $N = 2000$. Initially, all particles are assigned a zero displacement and a zero velocity except the center particle, which is given a nonzero kinetic energy $e(0)$ instead. Then absorbing boundary conditions are imposed, and after

a transient time of $2 \times 10^5$ we calculate $e(t)$, and the total energy remains in the chain at time $t$, up to $t = 8 \times 10^5$. We find that it decays as $e(t) \sim t^{-\lambda}$ [23] and that the exponent $\lambda$ depends on both the initial excitation energy $e(0)$ and $\gamma$: If $e(0)$ is small, harmonic behaviors manifest themselves, and $\lambda \to 0.5$, as pointed out in [31]. But for large enough $e(0)$ long-lived DBs may form, and thereby $\lambda \to 0$. Hence $\lambda \to 0$ is an indicator of the presence of long-lived DBs. We increase $e(0)$ progressively, and we find that it is exactly at $\gamma = \gamma_c$ when the signal of DBs first appears [see Fig. 5(b)], suggesting $e_{\rm sh}$ is smallest for $\gamma = \gamma_c$ and, accordingly, the concentration of the DBs is highest. [Note that the dependence of $e_{\rm sh}$ on $\gamma$ (not shown) is a smooth function with the minimum at $\gamma = \gamma_c$, consistent with the smooth dependence of $\alpha$ on $\gamma$ (see Fig. 2).]

In summary, we have studied a one-dimensional lattice of the FPU-$\beta$ type with both NN and NNN coupling. We find that, tuning the NNN coupling, the divergence exponent $\alpha$ of the heat conductivity may continuously change from 0.25 to about $\frac{1}{3}$, in contrast to the existence of a generality class(es). In addition, we have shown that there is a positive correlation between $\alpha$ and the energy of the in-band modes of DBs, on the basis of which we conjecture that the observed nonuniversal heat conduction behavior is due to the interactions between the in-band DBs and phonons. To establish a firm connection between them requires the details and direct evidence of the DB-phonon interactions, which are not provided in the present work.

We acknowledge the support by the NNSF (Grants No. 10805036, No. 10925525, No. 10975115, and No. 11147191), the SRFDP (Grant No. 20100121110021), and the start-up fund (Grant No. 022390) from Fuzhou University.

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