Dependence of thermal conductivity on discrete breathers in lattices

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We study the properties of heat conduction in chains of coupled particles subjected to different anharmonic on-site potentials. Particular emphasis is placed on the role of breathers in saturation of the thermal conductivity for chains with hard anharmonicity. When the chain particles are subject to on-site potentials with soft anharmonicity, we find a characteristic temperature, below which the conductivity decreases but while above which it increases. [S1063-651X(99)05912-7]

A general and challenging problem is to understand macroscopic phenomena and their statistical properties in terms of deterministic microscopic dynamics and, in particular, to connect macroscopic irreversibility with time reversible evolution of a system of interacting particles. There is still great interest in the properties of heat conduction in a chain of (linearly or nonlinearly) coupled nonlinear oscillators. Recent works [1–5] have aimed at obtaining, on a microscopic level, the Fourier heat law, according to which the heat flux through the chain is proportional to the temperature gradient (normal thermal conductivity). It is known that in integrable systems such as a harmonic chain [6], the Toda lattice, and others [4] a temperature gradient is not formed and therefore they do not obey the Fourier heat law. Nonintegrability is a necessary condition for a finite (normal) thermal conductivity. However, as shown recently for the Fermi-Pasta-Ulam [1] and the diatomic Toda chain [5], the existence of a temperature gradient does not necessarily mean the validity of the Fourier law. The nonintegrability of these systems leads to formation of a linear temperature gradient, but with a heat flux proportional not to N^{-1} but to $N^{-\alpha}$, $0 < \alpha < 1$, with N the chain length.

Other one-dimensional nonintegrable systems exist, however (so-called ding-a-ling [7] and ding-dong [8] models), that have a finite thermal conductivity. Recently [2], Hu, Li, and Zhao have found that in the Frenkel-Kontorova (FK) model a linear temperature gradient is formed and the heat flux is proportional to N^{-1}. Their general conclusion is that the phonon-lattice interaction is the key factor in the Fourier law, no matter whether the interparticle coupling in the FK model is harmonic or anharmonic.

The lack of details on the heat conduction mechanism in chains with on-site potentials provides a motivation for the present work. We will show that the anharmonicity of an on-site potential is a sufficient condition for finite thermal conductivity, no mather whether it is soft or hard. The behavior of thermal conductivity with temperature is studied for a number of standard on-site potentials, and we show that hard on-site anharmonicity leads to conductivity decrease with temperature. We explain this effect through nonlinear localized mode (discrete breather) formation, that accumu-

late the energy of thermal fluctuations and inhibit thermal transfer. A more detailed investigation of the behavior of the thermal conductivity with temperature in the FK model is also presented in our study.

We consider the Hamiltonian of harmonically coupled particles subject to an on-site potential in the following dimensionless form:

$$ H = \sum_n \left[\frac{1}{2} \dot{u}_n^2 + \frac{1}{2} (u_{n+1} - u_n)^2 + \omega_0^2 V(u_n) \right], \qquad (1) $$

where an overdot stands for differentiation with respect to dimensionless time t and $u_n = u_n(t)$ is the displacement of the nth atom of the chain from its equilibrium position. The on-site function $V(u)$ is normalized by $V''(0) = 1$, so that ω_0 measures the dimensionless eigenfrequency of a particle in the on-site potential. Besides the harmonic case with $V(u) = u^2/2$, this report will describe results for the sinh-Gordon (SHG) potential

$$ V(u) = \cosh u - 1 \qquad (2) $$

with hard anharmonicity, and two potentials with soft anharmonicity: the bounded single-well (BSW) potential

$$ V(u) = \frac{1}{2} (1 - \operatorname{sech}^2 u), \qquad (3) $$

representing a family of reflectionless potentials [9], and the periodic sine-Gordon (SG) potential (in the FK model)

$$ V(u) = 1 - \cos u. \qquad (4) $$

In order to study the heat conduction in a finite chain consisting of N particles, we split it into three segments, using the lateral segments with N_0 particles as thermal reservoirs (baths or thermostats) of the the Langevin type with different temperatures T_+ (left) and T_- (right). We choose the Langevin reservoir because of the recent study [3], according to which the Nosé-Hoover thermostat [10] appears
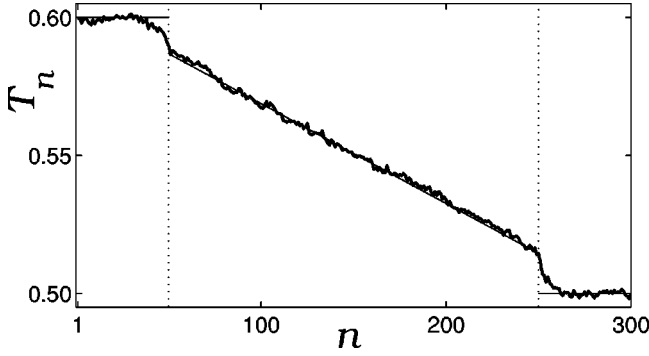
FIG. 1. Profile of local temperature T_n in the chain subjected to the SG potential ($N=300$, $N_0=50$, $T_+=0.6$, and $T_-=0.5$).

not to be appropriate for simulations of the thermodynamic limit. The corresponding equations of motion have the standard discrete form

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1} - V'(u_n)$$

for the internal segment ($n=N_0+1, \ldots, N-N_0$) and

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1} - V'(u_n) - \gamma \dot{u}_n + \xi_n^{\pm}$$

for the lateral segments with the "+" superscript for $n = N_0+1, \ldots, N-N_0$ and the "−" one for $n=N-N_0 +1, \ldots, N$. Here a prime stands for differentiation, γ is the relaxation coefficient, and $\xi_n^{\pm}$ is white noise driving the lateral segments and defined in the standard fluctuation-dissipation manner $\langle \xi_n^{\pm}(t) \rangle = 0$, $\langle \xi_n^+(t_1) \xi_n^-(t_2) \rangle = 0$, and $\langle \xi_k^{\pm}(t_1) \xi_l(t_2) \rangle = 2\gamma T_{\pm} \delta_{kl} \delta(t_1-t_2)$.

The system of equations of motion was integrated numerically. After thermal equilibrium was reached, the local temperature profile $T_n = \lim_{t \to \infty} (1/t) \int_0^t \dot{u}_n^2(\tau) d\tau$ and the local heat flux $J_n = \lim_{t \to \infty} (1/t) \int_0^t j_n(\tau) d\tau$ through the chain were established, where $j_n = \dot{u}_n(u_{n-1} - u_{n+1})/2$. The values $\omega_0 = 1$, $\gamma = 0.1$, $N_0 = 50$, and $N = 150, 200, 300, 500$ were used and the time of numerical integration was $t = 10^6$.

This method of thermalization allows us to introduce the boundary conditions properly. The local temperature profile T_n depicted in Fig. 1 shows that in the internal chain segment $N_0 < n \leq N-N_0$, transfer of thermal energy takes place. The temperature gradient has a linear form and the local heat flux does not depend on the specific chain site, i.e., $J_n = J$. This allows us to define the thermal conductivity

$$\kappa(N_1) = J N_1 / (T_{N_0+1} - T_{N-N_0}) \qquad (5)$$

with $N_1 = N - 2N_0$ being the length of the internal segment. The dependence of κ on N_1 for the three anharmonic on-site potentials (2), (3), and (4) is given in Table I. As follows from this table, for each anharmonic potential, doubling the length of the internal segment N_1 practically does not change $\kappa(N_1)$. Therefore, there exists a limit $\kappa = \lim_{N_1 \to \infty} \kappa(N_1)$ corresponding to the thermal conductivity κ at the mean temperature $T=(T_+ + T_-)/2$. Note that the thermal conductivity can also be found through the Green-Kubo formula

TABLE I. The thermal conductivity κ calculated according to Eq. (5) against the internal segment length N_1 ($T_+=0.6$ and $T_- =0.5$) and the conductivity κ_{GK} calculated according to the Green-Kubo formula (6) at $T=0.55$ for the chain with the three on-site potentials given by Eqs. (2), (3), and (4).

on-site potential	κ $N_1=50$	κ $N_1=100$	κ $N_1=200$	κ $N_1=400$	κ_{GK}
SHG	10.17	10.90	10.86	11.14	10.60
BSW	27.50	32.30	33.44	33.65	36.51
SG	17.33	17.43	18.26	18.31	17.66

$$\kappa = \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{NT^2} \int_0^t c(\tau) d\tau, \qquad (6)$$

where $c(t) = \langle J(0)J(t) \rangle$ is the correlation function of the total heat flux $J(t) = \Sigma_n j_n(t)$.

In order to find the function $c(t)$ in Eq. (6), we have considered a finite cyclic chain consisting of $N=2000$ particles, embedded into a Langevin bath. After the thermal equilibrium with the thermostat has been reached, the thermostat was removed and then the dynamics of the isolated chain was studied. To increase the accuracy of finding the correlation function, its averaged value was taken over 500 different realizations of initial thermalization of the chain. The numerical integration of the chain dynamics has shown that for each of the potentials (2), (3), and (4) at all values of temperature $T>0$, the correlation function $c(t)$ in the limit $t \to \infty$ tends to zero with exponential decay as illustrated in Fig. 2. The infinite integral in the Green-Kubo formula (6) converges and this results in finite values of thermal conductivity. The two ways of finding κ give very similar values as illustrated by Table I.

Consider now the dependence of the heat flux J on the temperature difference $\Delta T = T_+ - T_-$. To this end, we choose a finite chain of $N=300$ particles with zero temperature at the right end of the chain ($T_-=0$), so that $\Delta T = T_+$. The heat flux can be defined in another way, namely as the energy released at the right lateral segment due to the damping γ: $\bar{J} = \gamma \Sigma_{n=N-N_0+1}^N T_n$. The numerical integration of the equations of motion confirms that $\bar{J}$ equals the heat
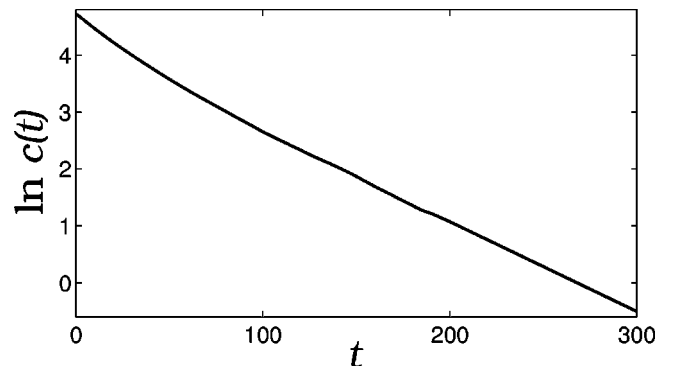

FIG. 2. Time dependence of the natural logarithm of the correlation function $c(t)$ calculated at the mean temperature $T=(T_+ +T_-)/2=0.55$.
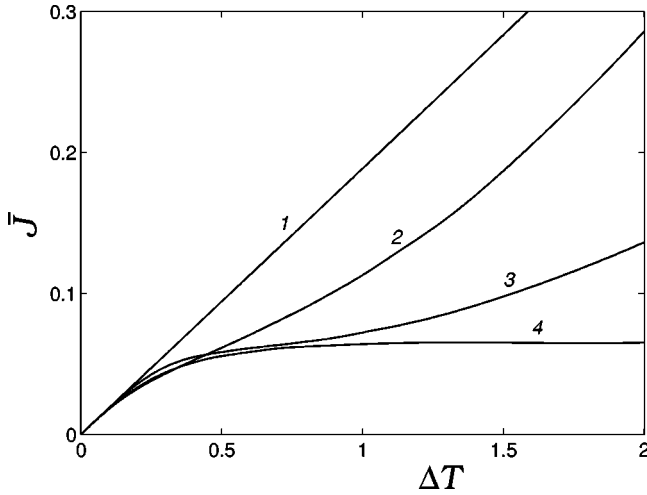
FIG. 3. Dependence of the heat flux $\bar{J}$ on temperature difference $\Delta T = T_+ - T_-$ in the chains with the harmonic (curve 1), the soft BSW (curve 2), soft SG (curve 3), and hard SHG (curve 4) on-site potentials ($N=300$, $N_0=50$, $T_+ = T$, and $T_- = 0$).

flux in the internal region of the chain: $J_n = \bar{J}$, $n = N_0 + 1, \ldots, N - N_0$.

The dependence of the heat flux $\bar{J}$ on the temperature difference ΔT is presented in Fig. 3. As can be seen from this figure, the magnitude of the heat flux increases monotonically with temperature. In the chain with the harmonic on-site potential the heat flux is proportional to temperature. This is due to the fact that in the linear chain the Fourier law is not established but the chain attains throughout (except in the contact points) the average contact temperature [6]. The anharmonicity of the potential results in slowing down the increase of the heat flux. For the potentials BSW and SG with soft anharmonicity, this decrease becomes maximal at $\Delta T = 0.5$ that corresponds to the binding energy of the chain with the substrate formed by the on-site potentials. However, further increase of temperature leads to increasing the speed of growth: Disconnection of the chain from the substrate occurs and in the high-temperature limit the chain becomes isolated. Completely different behavior is observed in the chain with the hard anharmonic potential (2). Here, at $\Delta T \to \infty$ the heat flux $\bar{J}$ tends to a finite value: a saturation occurs because the magnitude of the flow cannot exceed a certain maximal value.

In order to clarify the saturation effect in chains with hard anharmonicity, we note that in addition to extended linear small-amplitude oscillations (phonons), nonlinear large-amplitude strongly localized modes (so-called discrete breathers; for a review see Ref. [11]) can exist in the chain. In order to investigate the role of breathers on the thermal conductivity, we calculate the power-density spectra of thermal fluctuations for different types of anharmonicity. For the chain with the harmonic on-site potential, this spectrum is given analytically: $E(\omega) = 2\omega / \pi \sqrt{(\omega^2 - \omega_0^2)(\omega_1^2 - \omega^2)}$, $\omega_0 < \omega < \omega_1$, where ω_1 is the upper edge of the phonon band, $\omega_1^2 = \omega_0^2 + 4$, and depicted by curve 1 in Fig. 4(a).

This figure also represents the typical power spectra calculated numerically in the case of hard anharmonicity given by Eq. (2). At low temperature ($T = 0.05$), the spectrum of (small-amplitude) anharmonic thermal fluctuations practi-
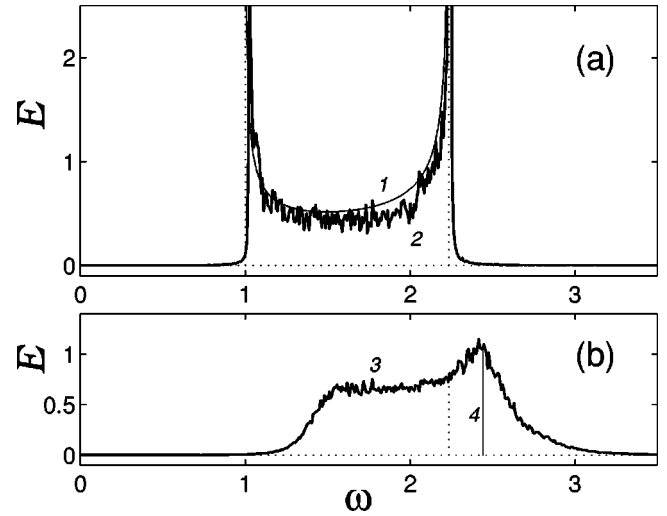

FIG. 4. Power spectra of thermal fluctuations $E(\omega)$ in the chains with harmonic and hard anharmonic on-site potentials. (a) Analytical form of the spectrum for the harmonic chain (curve 1) given for comparison with a typical realization of the spectrum computed numerically at temperature $T = 0.05$ for the chain with the hard SHG anharmonicity (curve 2). (b) A typical realization of the spectrum computed numerically at $T = 2.05$ (curve 3). Line 4 represents the breather frequency $\omega_b(T)$ that corresponds to the position of the peak in the spectrum.

cally coincides with that in the chain with the harmonic potential (compare curves 1 and 2). However, for high temperature ($T = 2.05$), the spectrum is shifted to the high-frequency region as illustrated by Fig. 4(b). In addition to phonons, in this spectrum there exist high-frequency localized nonlinear oscillations, discrete breathers, whose frequency exceeds ω_1. The energy of a breather E_b monotonically increases while its width D decreases with increase of the frequency. From the equation $E_b(\omega) = 2TD(\omega)$ one can determine the frequency $\omega_b(T)$, at which the energy distribution in the breather localization region corresponds to the energy level of thermal fluctuations. The breathers with this frequency should have the greatest probability of formation in the thermalized chain. Therefore, as clearly demonstrated by Fig. 4(b), the power spectrum has a maximum at this frequency. At $T = 2.05$ more than half the total energy is in thermal oscillations with frequency $\omega > \omega_1$. Thus, one can conclude that there is a large contribution of breathers to thermal capacity of the chain at high temperatures. For hard anharmonicity of the on-site potential, the breathers appear to be strongly localized *standing* oscillations. They cannot contribute to transfers of thermal energy and, as a result, thermalization of breathers results in an effective reduction of thermal conductivity of the chain.

In order to show the presence of high-frequency standing breathers in a thermalized chain, let us consider the time evolution of the thermalized chain with the initial temperature $T = 2.05$. We chose a finite chain consisting of $N = 500$ particles and place it in the Langevin heat bath. After the thermalization of the chain is complete, we removed the bath, but introduced some damping at the chain ends [12]. Such a numerical integration of the equations of motion has shown that after absorption of all *mobile* excitations by the chain ends, in the internal segment of the chain, a standing
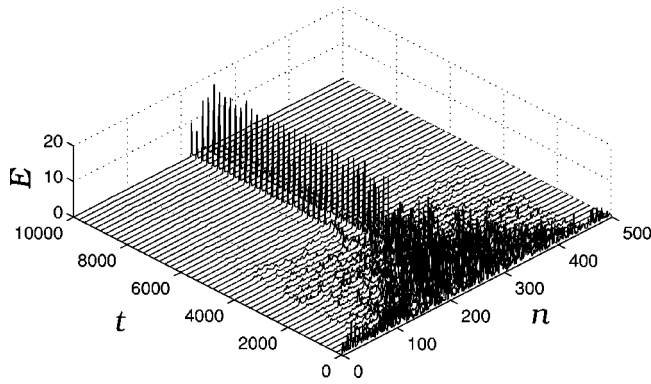
FIG. 5. Formation of a standing breather from thermal fluctuations of the chain. Initially (at $t=0$), the temperature of the chain was $T=2.05$. In order to avoid reflection effects, the chain ends include damping ($N=500$, $N_0=50$, and $T_+=T_-=0$).

FIG. 6. Thermal conductivity κ against the mean temperature T of the chains with the soft BSW (curve 1), soft SG (curve 2), and hard SHG (curve 3) on-site potentials.

breather still appeared to be present as illustrated by Fig. 5, this is in agreement with Peyrard's study [13].

Dependence of the thermal conductivity κ on the mean temperature of the chain $T=(T_++T_-)/2$ is presented in Fig. 6. In the chains subjected to the BSW and SG potentials for $T<0.55$ the conductivity κ monotonically decreases with increase of temperature. At $T=0.55$, a minimum is reached and further temperature increase leads to augmentation of κ. At $T=0.55$, the energy of thermal fluctuations becomes greater than the binding energy of the chain with the substrate. The chain becomes increasingly disconnected from the substrate, so that in the limit of high temperatures it acquires the infinite conductivity of an isolated harmonic chain. In the chain with the hard SHG potential, disconnection of the chain from the substrate is impossible. In this case, the contribution of high-frequency standing breathers in the chain thermalization, which prevent the heat conduction, rapidly increases with temperature. As a result, the increase of temperature results in a monotonic decrease of the thermal conductivity; $\kappa\to 0$ if $T\to\infty$. This result is in good agreement with the effect of saturation of heat conduction demonstrated by curve 4 in Fig. 3.
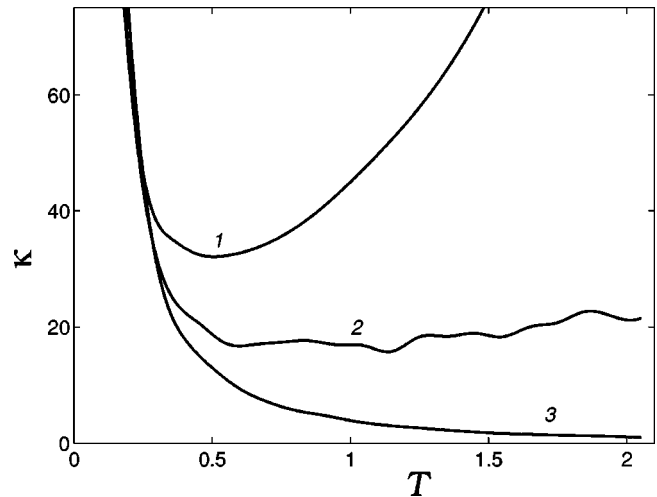
In conclusion, we have shown that a chain of coupled particles each of which is subject to an *anharmonic* on-site potential, independently of the sign of anharmonicity, has a finite (i.e., normal) heat conduction. In the presence of hard anharmonicity (as in the SHG model), the thermal conductivity tends monotonically to zero with increasing of temperature. This phenomenon is connected with thermalization of high-frequency *standing* breathers. When the chain particles are subject to a *bounded* on-site potential (which necessarily contains soft anharmonicity), there exists a critical value of temperature T_c corresponding to the binding energy of the particles with the on-site (substrate) potential. At $T<T_c$, the thermal conductivity monotonically decreases with temperature, while at $T>T_c$ it increases monotonically, and at $T=T_c$, the chain becomes disconnected from the substrate.

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