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Effect of dynamical localization on negative differential thermal resistance

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HIGHLIGHTS

- Understand NDTR based on the analysis of vibration spectra.
- Theoretical analysis is proposed for effects of dynamical localization on NDTR.
- Presence of NDTR is explained from a microscopic viewpoint.

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ABSTRACT

We numerically study heat conduction in a homogeneous lattice of interacting oscillators via analyzing the power spectrum of system's vibrations. The mechanism for the presence and the size effect of negative difference thermal resistance (NDTR) is understood based on dynamical localization of phonon modes. Localized modes are clearly shown in the spectra when large temperature difference is applied to the system. And then we propose a quantitative analysis for the relation between NDTR and the localization in a phenomenological way, which indicates that NDTR can be obtained in a small system with system size less than the localization length and explain the saturation of heat flux. The theoretical calculations are consistent with numerical simulations.

1. Introduction

In recent years, much effort has been devoted to heat conduction in low-dimensional dynamical systems from both theoretical and experimental aspects [1,2]. An interesting problem lies in deriving Fourier's law on purely dynamical grounds without recourse to any statistical hypothesis. A complete theory to bridge microscopic dynamics, such as dynamical localization, and macroscopic energy transport is still lacking in spite of relevant progress. On the other hand, heat conduction in low-dimensional systems also has practical implications through manipulating heat flow on the nanoscale and processing information by utilizing phonons [3].

As we all know, the inventions of electrical devices that control the electric flow have lead to an impressive technological development in modern electronics. However, a similar technology based on electronic analogs via control heat flow has not yet been realized. Significantly, the thermal counterpart of some electric devices, such as thermal diode [4–7], thermal transistor [8], thermal logic gates [9] and thermal memory [10] has been theoretical studied in dynamical models recently. Negative differential thermal resistance (NDTR), i.e., the counterintuitive phenomenon of decreasing heat flux for increasing

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temperature difference, plays a key role in the operation of some model thermal devices [8–13], which is reminiscent of the role of negative differential electrical resistance (NDER) in the operation of the tunnel diode [14] and of some other electrical devices [15]. In light of the importance of NDTR to design thermal devices and the role of NDER in modern electronics, much interest has been in understanding the physical mechanism of NDTR. In particular, studies have been carried out for various nonlinear oscillator systems, namely, the Frenkel–Kontorova model [16–18], ϕ^4 model [19,17] and the Fermi–Pasta–Ulam model [17]. The mechanism of NDTR for systems of coupled segments lies in the temperature dependent overlap of phonon spectra of each segment [16,19]. However, it is not applicable to explain the size effect of NDTR and the occurrence of NDTR in a one-dimensional homogeneous lattice. A phenomenological approach is recently proposed to give the conditions for the occurrence of NDTR generally in a homogeneous model and explain its size effect via a macroscopic way [17,20]. Unfortunately, the mechanism of NDTR from a *microscopic* viewpoint is so far unavailable. In this paper, we will propose a new way to understand NDTR based on the dynamical localization of oscillation modes [21], which are shown to affect energy transport in nonlinear lattices [22–25]. The approach can explain the presence of NDTR in a nonlinear homogeneous lattice as well as its size effect from a microscopic viewpoint. Particularly, we analyze the power spectrum of vibrations of the ϕ^4 lattice under different temperature differences, and observe the presence of the intrinsic localized modes. In addition, we propose a theoretical analysis for the energy transport via the localized modes, which is consistent with numerical simulations.

2. Model and results

The homogeneous lattice model can be generally described by a Hamiltonian of the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(x_i - x_{i+1}) + U(x_i), \tag{1}$$

where N is the total number of particles (i.e., system size), and p_i is the instantaneous momentum, x_i is the deviation from its equilibrium position of the ith particle, m is the mass, $V(x_i - x_{i-1})$ is the nearest-neighbor interaction potential, and $U(x_i)$ is the on-site potential, respectively. In the present study, we mainly consider a specified model, i.e., ϕ^4 model, in which $V(x)$ is given by the harmonic potential,

$$V(x) = \frac{1}{2}kx^2, \tag{2}$$

and $U(x)$ is given only by an unbounded nonlinear on-site potential of the form

$$U(x) = \frac{1}{4}\lambda x^4. \tag{3}$$

Here k is the coupling constant and λ is the nonlinear strength of the on-site potential.

In order to form a stationary heat flux, the end particles $i = 1$ and $i = N$ are connected to Langevin heat baths [1] at temperatures T_+ and T_-, respectively. The equations of the motion then take the form

$$m\ddot{x}_i = -\frac{\partial H}{\partial x_i} - \gamma_i \dot{x}_i + \eta_i, \tag{4}$$

where $\gamma_i = \gamma(\delta_{i,1} + \delta_{i,N})$ and $\eta_i = \eta_+\delta_{i,1} + \eta_-\delta_{i,N}$. The noise terms $\eta_\pm(t)$ denote a Gaussian white noise that has a zero mean and a variance of $2\gamma k_B T_\pm$, γ is the friction coefficient and k_B is Boltzmann's constant. Both the mass m and Boltzmann's constant k_B are set as units. In our simulations, fixed boundary conditions are used, i.e., $x_0 = x_{N+1} = 0$ and the equations of motions are integrated by the second-order stochastic Runge–Kutta algorithm [26] with a small time step $h = 10^{-3}$. The local heat flux is defined by $j_i = \langle \dot{x}_i F(x_i - x_{i-1}) \rangle$ [1] and the local temperature is defined by $T_i = \langle \dot{x}_i^2 \rangle$, where $a = 1$ is the lattice constant and the notation $\langle \ldots \rangle$ stands for a time average after the system reaches a nonequilibrium steady state.

Q3 Fig. 1 shows a typical plot of NDTR exhibited in the ϕ^4 model when the system size is small [17]. In this case there exists a critical temperature difference ΔT^*, which separates the low-ΔT regime of positive differential thermal resistance (PDTR) and high-ΔT regime of NDTR. When system size is large ($N = 512$), the heat flux approaches to a constant as ΔT increases, i.e., NDTR regime disappears [17,18]. As illustrated in Fig. 2, the slope of heat flux in NDTR regime (the green line in Fig. 1) tends to zero while ΔT^* has a nonmonotonic variation as N increases. The phenomenon resistive phase change from NDTR to PDTR is also predicted in mass graded system, which is caused by the vibrational spectra mismatched or matched [27,28].

To understand the microscopic mechanism underlying the phenomenon, we analyze the power spectrum of the time series of the particles' instantaneous momentum $p_i(t)$ by fast Fourier transformation. During the FFT, the time series' length of each particle is 2^{11} and the sample interval $\triangle = 200h$, where h is the time step for the integration. As shown in Fig. 3(a) and (c), the power spectrum is an almost parallel strip for the case of small temperature difference, which corresponds to PDTR. While the power spectrum looks like a taper for the case of large temperature difference (see Fig. 3(b)), for which NDTR occurs. From the viewpoint of dynamical localization, the frequency of nonlinear oscillators relies on the amplitude of oscillation or, equivalently, the input energy due to the existence of the nonlinearity [21]. In the low-ΔT case, the energy of each oscillator is almost the same, thus they oscillate in the same frequency range. Therefore, there may exist resonance

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