Physica A 433 (2015) 9–16

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Phononic heat transfer through a one dimensional system subject to two sources of nonequilibrium

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HIGHLIGHTS

- Energy transfer in systems subject to different sources of nonequilibrium is studied.
- Single and multiple resonant phenomena depending on the frequency regimes are found.
- A crossover between a mechanical resonance and a thermodynamical one is reported.
- A "red shift" resonance that is size dependent is shown.

ARTICLE INFO

Article history:
Received 14 November 2014
Received in revised form 16 March 2015
Available online 1 April 2015

Keywords:
Transport processes
Heat conduction
FK lattices

ABSTRACT

We analyze the energy transport in a one dimensional chain composed by two Frenkel–Kontorova (FK) segments connected together by a time modulated coupling. The ends are immersed in two thermal reservoirs with oscillating temperatures. We observe a single and multiresonant heat transport depending on the regimes considered, with a crossover between a mechanical resonance and a thermodynamical resonance. The dynamical tuning between these two regimes requires the synergetic presence of both time dependent sources of nonequilibrium. In the single resonant regime we analyze a "red shifted" resonant frequency that is dependent on the size of the system.

1. Introduction

During last years a fast development of the emerging field of *phononics* was achieved, where the manipulation and control of phonons (heat transfer) at the nanoscale and molecular level has become a fundamental topic due to its technological and practical implications [1]. The problem of phonon transport, that is a thermal nonequilibrium problem, is less understood than that of electron transport. In addition to electrons and photons, phonons carry heat and information. However, comparing with electron and photons, phonons are more difficult to control. So, an important and relevant issue is to understand further the mechanisms for heat transfer assisted by phonon and its generation in nano and micro devices and how it affects their structural stability. In this sense, it becomes essential to study mechanisms that dissipate or redirect heat efficiently, or under what operating conditions a given device can act as a good conductor or insulator.

It is known that two necessary conditions are fundamental for the emergence of thermal current: symmetry breaking and nonequilibrium sources. These two conditions in nonlinear lattices produce abnormal thermal transport phenomena, such as thermal rectification and negative differential thermal resistances.

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http://dx.doi.org/10.1016/j.physa.2015.03.024
0378-4371/

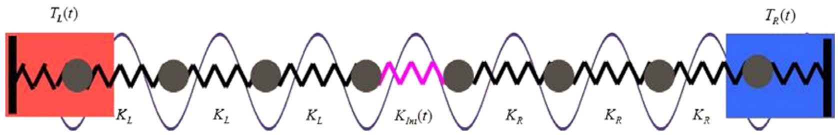

Fig. 1. Model system composed by two one-dimensional chains coupled by a modulated interaction in time and coupled to two heat baths Langevin at their ends.

Several models and mechanisms have been proposed to control or manipulate the heat at the nanoscale. One way is to tune the structural asymmetry or the degree of anharmonicity [2–11]. It has been demonstrated that the nonlinearity can be utilized to design novel nanoscale solid-state thermal devices such as thermal diodes [12–16], thermal transistors [17], thermal logic gates [18] and thermal memories [19,20].

Other mechanisms may require an external applied work on the system tuning or controlling heat *dynamically*. In Ref. [14] it was proposed a heat ratchet to direct heat flux from one bath to another in a nonlinear lattice, which periodically adjusts two baths temperatures while the average remains equal, or brownian heat motors to shuttle heat across the system [21]. We can also mention heat pumps which directs heat against thermal bias in nanomechanical systems [22], or phonon pumps induced at the molecular levels by an external force or with a mechanical switch on–off or a modulation of the coupling between different parts of the system [23–26]. Experimentally this can be done in molecular junctions or in molecular systems, for example, varying the distance among them. It was also demonstrate theoretically that mechanical actions as stretching (or compressing) a wire, can tuned the phononic band structure in such a way that multiple phononic channels are opened one by one. In this way and as in the electronic case, it is found a multiple-step quantized phononic thermal conductance [3].

The distinctive and unique transport properties of low-dimensional system has posted great challenge to find mechanisms to manipulate heat transfer in meso and nanoscopic phonon systems. Therefore, it is highly desirable any attempt towards a thorough understanding of the heat transport in general one-dimensional nonlinear lattice systems. In this paper we extend these studies to analyze the synergetic effect of heat transfer through one dimensional systems when are present simultaneously two time dependent mechanical and thermodynamical sources of nonequilibrium.

2. The model

We consider a one dimensional array of atoms, harmonically and bidirectionally coupled. The chain is divided in two segments (L, R) with different coupling intensities K_L and K_R between elements and coupled together also harmonically with a coupling constant K_{int}. The system is subject to an on-site potential (Frenkel–Kontorova (FK) chains) as it is shown in Fig. 1.

The Hamiltonian of the system can be written as: $H = H_L + H_{int} + H_R$ where $H_{L/R}$ is the Hamiltonian to the left (L)/right (R) segments respectively and H_{int} represents the interaction between the two segments.

$$H_{L/R} = \sum_{i=1}^{N} \frac{P_i^2}{2m_i} + \frac{1}{2}K_{L/R}(X_{i+1} - X_i)^2 - \frac{V_o}{4\pi^2}\cos(2\pi X_i) \tag{1}$$

with N the total number of atoms.

If each segment has $N/2$ elements, the interaction Hamiltonian can be written as:

$$H_{int} = \frac{1}{2}K_{int}(t)(X_{N/2+1} - X_{N/2})^2 \tag{2}$$

with m_i the mass of the ith atom, $X_i = q_i - ia$ denotes the displacement from the equilibrium position ia, where a is the periodicity of the on-site potential (corresponding to a commensurate state), and P_i is the momentum.

$K_{L/R}$ are the elastics constants in each segments and V_0 is the depth of the on-site potential. The fixed ends of the L/R segments are in contact with two thermal baths which are simulated through Langevin type reservoirs with zero mean and variance $\langle \xi_i(t), \xi_k(t') \rangle = 2\gamma K_B T_i \delta(t - t')\delta_{i,j}$, where γ is the strength of the coupling between the system and the baths, and T_i, $i = L/R$, is the temperature of each bath. The system is driven out of equilibrium by two different mechanisms:

(a) Modulation of the coupling between segments: $K_{int}(t) = K_0(1 + \sin(\omega_K t))$.
(b) Modulation of the temperature of the reservoirs: $T_{L,R}(t) = T_{0,i}(1 + \Delta sgn(\sin(\omega_{temp} t)))$, $i = L, R$ with $T_{0,i}$ the reference temperature of each reservoir.

The integration of the equations of motion is performed with a 2nd-order stochastic Runge–Kutta algorithm, for sufficiently long time (of order of 10^9–10^{10} integration steps) to guarantee that the system reaches a stationary state. We apply fixed boundary conditions and for the numerical simulations we use dimensionless parameters: spring constants K_i in units of K_R, moments in units $[a(mk_R)^{1/2}]$, frequencies in units $[(K_R/m)^{1/2}]$ and temperatures in $[a^2K_R/k_B]$. For a typical atom and a typical situation these units corresponds to frequencies $\sim 10^{13}$ s^{-1} and temperatures $\sim 10^3$, 10^4 K. Thus the nondimensional temperatures 0.01–0.1 correspond to temperatures of the order 100–1000 K. On the other hand, frequencies are assumed to be smaller than the inverse of typical electron–phonon relaxation times $\sim$0.1 ps (dephasing time), in order to consider only the relevant time scales of phonon scattering processes.