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Frequency thermal response and cooling performance in a microscopic system with a time-dependent perturbation

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HIGHLIGHTS

- Energy transfer in systems subject to time dependent perturbations is studied.
- Frequency dependent heat transport regimes are studied.
- Characterization of the cooling performance of the system.

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ABSTRACT

Following the nonequilibrium Green's function formalism we study the thermal transport in a composite chain subject to a time-dependent perturbation. The system is formed by two finite linear asymmetric harmonic chains subject to an on-site potential connected together by a time-modulated coupling. The ends of the chains are coupled to two phononic reservoirs at different temperatures. We present the relevant equations used to calculate the heat current along each segment. We find that the system presents different transport regimes according the driving frequency and temperature gradients. One of the regimes corresponds to a heat pump against thermal gradient, thus a characterization of the cooling performance of the device is presented.

1. Introduction

Nowadays, the technological implementations in the meso and nanoscale require the management of substantial energies that can be generated, becoming harmful for a device. So significant improvements are needed in the direction of controlling energy, and thus heat, to avoid structural damages. However, many studies show that the management of heat can also display intriguing features which allow the design of devices with novel operating regimes [1,2].

Spontaneously heat flows from objects at high temperatures to objects at lower temperatures. However heat pumps enable heat to flow against temperature gradient by means of an applied external work. At the meso and nanoscale several interesting applications have been developed in molecular electronics, thermometry and thermal machinery [3–5]. Many models of heat pumps have been proposed based on different mechanisms such as heat ratchets that periodically adjust two baths' temperatures while the average remains equal, brownian heat motors to shuttle heat across the system [6], heat pumps which direct heat against thermal bias in nanomechanical systems [7]. At molecular levels phonon pumps can

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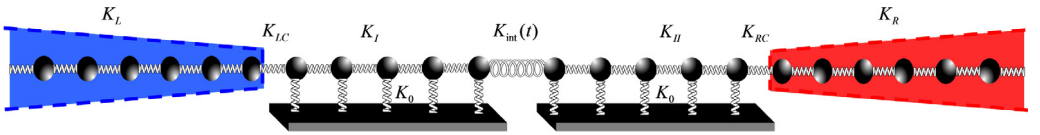

Fig. 1. Sketch of the microscopic model. The system is composed by two one-dimensional chains of particles coupled by a modulated interaction in time. The semi-infinite left chain is kept at a temperature T_L and the semi-infinite right one at T_R.

also be induced by an external force or by mechanical switch on–off of the coupling between different parts of the system [8–14]. Experimentally the last can be done in molecular junctions or in molecular systems, for example, varying the distance among them or applying stretchings and compressions.

Cooling is another relevant feature because of applications in the quantum realm. Experimental implementations of quantum refrigerators have been developed based on electronic devices in the presence of ac driving fields [15–18], absorption of phonons (heat) with electrons using nanomechanical devices or active feedback for cooling nanomechanical cantilevered beams [19–22]. In turn models based on pumping phenomena have been proposed as moving barriers in a cavity to pump phonons from a cold reservoir to a hotter one, or driven two level systems or molecular junctions in contact with phononic baths [23,24]. In the present work, the mechanism underlying cooling is mainly the phonon manipulation that can work both in insulators and electrical conductors, unlike the electronic cooling where charge, spin and coherence are important.

We present a microscopic model of a phonon pump based on a time dependent modulation of the contact between two one dimensional components. We show that this system can work not only as a heat engine, but it can also operate as a phononic refrigerator.

The paper is organized as follows. In Section 2 we present the microscopic model. In Section 3 we describe the theoretical framework and methodology used to solve numerically the problem. In Section 4 we present the different regimes for heat transport, discussing the role of external frequency and the size of system. In Section 5 we analyze the cooling regime comparing with the optimal case. Section 6 is devoted to summarize the results.

2. The model

We propose a microscopic model for energy transport assisted by acoustic phonons. We consider a one dimensional array of atoms, harmonically and bidirectionally coupled, sketched in Fig. 1. The central chain is divided in two segments I (left) and II (right) with different coupling intensities K_{I} and K_{II} between identical atoms or molecules (referred as "masses") and coupled together also harmonically with a coupling constant $K_{int}(t)$. The system is subject to a local harmonic pinning potential and connected to L (left end) and R (right end) semi-infinite chains of masses m_L and m_R respectively, coupled harmonically by spring constants K_L and K_R. This chains play the role of phonon reservoirs with temperatures T_L and T_R. We assume that the system can only vibrate longitudinally that is, we are modeling a heat pump assisted only by longitudinal acoustic modes.

The Hamiltonian of the system can be written as: $H = H_L + H_R + H_{central} + H_{int}(t) + H_{contact}$ where $H_{L,R}$ are the Hamiltonians of the left (L)/right (R) reservoirs respectively, $H_{central}$ describes the contributions of the segment I and the segment II of the central chain, H_{int} represents the interaction between them and $H_{contact}$ represents the contact between the central chain and the reservoirs.

$$H_{central} = \sum_{\alpha=I,II} \sum_{i=1}^{N_\alpha - 1} \frac{p_{i,\alpha}^2}{2m_{i,\alpha}} + \frac{1}{2} K_\alpha (x_{i+1,\alpha} - x_{i,\alpha})^2 + \frac{1}{2} K_0 x_{i,\alpha}^2 \tag{1}$$

with N_α the total number of particles.

The two segments $\alpha = I, II$ of the central chain have equal length $N_\alpha = N/2$. K_α are the elastics constants in each segment and K_0 is the spring constant of the local pinning potential. They are harmonically coupled with a time dependent strength $K_{int}(t) = K_{int}^0 + K_{int}^1(t) = K_0 + K_{int}\cos(\omega_0 t)$, where K_0 is the static contribution. K_{int} and ω_0 are the amplitude and frequency of the time-modulated parts respectively.

Thus the interaction Hamiltonian can be written as:

$$H_{int} = \frac{1}{2} K_{int}(t)(x_{N_1,I} - x_{N_1,II})^2 \tag{2}$$

with $m_{i,\alpha}$ the mass of the ith atom in the chain α, $x_{i,\alpha} = q_{i,\alpha} - ia$ denotes the displacement from the equilibrium position ia, where a is the equilibrium distance between particles and $p_{i,\alpha}$ is the momentum. The index $i = 1$ labels the atom of a segment that is in contact with a reservoir

The reservoir Hamiltonians corresponding to the semi-infinity chains are

$$H_\beta = \sum_{i=1}^{N_\beta} \frac{p_{i,\beta}^2}{2m_{i,\beta}} + \frac{1}{2} K_\beta (x_{i,\beta} - x_{i+1,\beta})^2 \tag{3}$$

with $N_\beta \to \infty$ ($\beta = L, R$) number of particles.