Physica E 67 (2015) 112–115

Contents lists available at ScienceDirect

Physica E

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

Transmission of longitudinal phonons through a mass-spring nanoring

Hassan Rabani [a,b,*], Mohammad Mardaani [a,b]

[a] Department of Physics, Faculty of Sciences, Shahrekord University, P. O. Box 115, Shahrekord, Iran
[b] Nanotechnology Research Center, Shahrekord University, 8818634141 Shahrekord, Iran

HIGHLIGHTS

- Coherent phonon transport through an extended cyclic mass-spring structure.
- Assumption of harmonic approximation and longitudinal in-plane vibrations.
- Using Green's function method to compute the phononic transmission and DOS.
- A hexagonal mass-spring ring in the presence of a massive mass as an example.

ARTICLE INFO

Article history:
Received 22 June 2014
Received in revised form
19 November 2014
Accepted 25 November 2014
Available online 29 November 2014

Keywords:
Phonon transmission
Nanoring
Harmonic approximation
Green's function

ABSTRACT

In this paper, we study the coherent phonon transport through a cyclic mass-spring structure which is embedded between two longitudinal phononic leads within the harmonic approximation. We assume only the in-plane vibrations for the atoms of the structure and also the nearest neighbor interaction between them. By starting from the system potential energy and then using the Green's function method, we construct a formalism to compute the phononic transmission coefficient and density of states/modes of the system. The numerical calculations are performed for a hexagonal mass-spring ring in the presence and absence of a massive impurity. The results reveal that, the variation of value of the masses or spring constants in the ring leads to appearance of the Fano resonance in the transmission spectrum. This phenomenon occurs at a special phonon frequency independent of the impurity position in the structure.

1. Introduction

The experimental challenges have made that the study of thermal properties of nano-devices has been investigated less than the electrical ones by the scientists [1,2]. However, the recent high-rapidly developments in nanofabrication and measurement technologies, enables us today to study experimentally the thermal properties of nanostructures [3,4]. For instance, thermal rectifiers [5], transistors [6], switches [7,8], and memories [9] have been experimentally demonstrated. Also the size and geometry dependent [4,10], electron–, magnon– and phonon–phonon scattering and related phenomena [11–13] in heat transport, have theoretically been illustrated in the recent publications. Therefore, this field attracted the attention of researchers on this research area in both experimental and theoretical viewpoints. On the other hand, in the field of micro- and nano-electronics, the influence of heat dissipation and transport on electronic responses of the system is an important issue. The thermal properties of a structure are originated mainly from the electrons and atomic vibrations. Indeed, the consideration of these contributions even separately helps us to understand the underlying physics and mechanisms of the thermal phenomena.

Since, a significant amount of thermal conductance of molecular structures, originates from phononic contribution, therefore the calculation of phonon transmission coefficient becomes necessary. By means of this quantity the computation of other thermodynamic quantities like Seebeck coefficient [14], Raman response coefficient [15], and specific heat [16], is possible.

In this paper, we study the problem of phonon transport through a cyclic molecule including one or none impurity embedded between two simple phononic leads. We replace the molecule bonds by springs and allocate them to the corresponding spring constants in order to construct a simple mass-spring model. We also suppose the atomic displacements are in the bond directions and we employ the Green's function technique within the

* Corresponding author at: Department of Physics, Faculty of Sciences, Shahrekord University, P. O. Box 115, Shahrekord, Iran.
E-mail addresses: rabani-h@sci.sku.ac.ir (H. Rabani), mohammad-m@sci.sku.ac.ir (M. Mardaani).

http://dx.doi.org/10.1016/j.physe.2014.11.020
1386-9477/

harmonic approximation. In this manner, we insert the effect of phononic leads as self-energies in the phonon Green's function. Then, the phononic transmission and density of modes are evaluated by using the system Green's function. Depending on the position of impurity and output lead contact as well as bond structure of the molecule, there are some constructive and destructive interferences which lead to interesting phenomena such as Fano and anti-resonances in the system phononic spectra.

This paper is organized as follows. In Section 2, we present the harmonic model, the system geometry and the Green's function model in order to formulate the phonon transmission coefficient and density of modes for the present system. These quantities are calculated numerically for some different configurations and situations in Section 3. We also discuss and compare the numerical results in this section. We conclude the paper in Section 4.

2. Model and formalism

We consider a mass-spring benzene-like molecule embedded between two similar semi-infinite phononic leads within the harmonic approximation. We label atoms in the center ring according to Fig. 1. We indicate all force-constants, in the left (L) and right (R) leads by C_s. We assume the Kekulé-like structure for the ring including two different bands with different spring constants. So, the corresponding spring constant for *single* and *double* bonds are represented by C_s and C_d, respectively. In the harmonic approximation, the potential energy of the system reads

$$U = \sum_{i<j} U_{ij} = \frac{1}{2}\sum_{i<j} C_{ij}\left(\hat{n}_{ij}\cdot(\vec{r}_i - \vec{r}_j)\right)^2, \tag{1}$$

where U_{ij} is the potential energy between i-th and j-th masses, C_{ij} can take the values C_s or C_d, $\hat{n}_{ij}$ is the unit vector in the $i-j$ bond direction; and finally $\vec{r}_{i(j)}$ is the *in-plane* vector displacement from equilibrium position of $i(j)$-th atoms. For an extended hexagonal mass-spring ring depicted in Fig. 1, the explicit forms of U_{ij} are

$$U_{01} = \tfrac{1}{2}C_s x_1^2, \tag{2b}$$

$$U_{12} = \frac{1}{2}C_s\left(\frac{1}{2}(x_1 - x_2) + \frac{\sqrt{3}}{2}(y_1 - y_2)\right)^2, \tag{2c}$$

$$U_{23} = \frac{1}{2}C_d(x_2 - x_3)^2, \tag{2d}$$

$$U_{34} = \frac{1}{2}C_s\left(\frac{1}{2}(x_3 - x_4) - \frac{\sqrt{3}}{2}(y_3 - y_4)\right)^2, \tag{2e}$$

$$U_{45} = \frac{1}{2}C_d\left(\frac{1}{2}(x_4 - x_5) + \frac{\sqrt{3}}{2}(y_4 - y_5)\right)^2, \tag{2f}$$

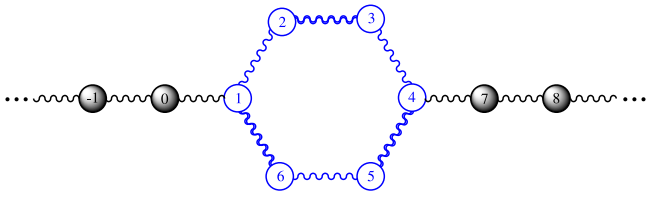

Fig. 1. A benzene-like ring connected to two simple mass-spring chains. The corresponding springs of the single and double bonds are represented by solid and bold-solid wavy lines, respectively. The numbers show the labels of the atoms in the hexagonal ring and leads.

$$U_{56} = \frac{1}{2}C_s(x_5 - x_6)^2, \tag{2g}$$

$$U_{61} = \frac{1}{2}C_d\left(\frac{1}{2}(x_3 - x_4) - \frac{\sqrt{3}}{2}(y_6 - y_1)\right)^2, \tag{2h}$$

$$U_{47} = \frac{1}{2}C_s x_4^2, \tag{2i}$$

The inverse Green's function matrix of the ring in the presence of phononic leads is

$$G^{-1} = (m\omega^2 - \Sigma_L\delta_{i,1} - \Sigma_R\delta_{i,2nf-1})I - A, \tag{3}$$

where ω is frequency of the incident phonon from leads, m is the mass of each atom, $\Sigma_{L(R)}$ is the self-energy of the ring due to the existence of left (right) for which the explicit form will be given later. Here, I is the unit matrix with dimension $2N\times 2N$ and $\delta_{i,j}$ refers the Kronecker delta. We assume that one lead is attached to the ring from first atom and another is connected via the atom number n_f of the ring. Moreover, A is the force-constant matrix with the following elements

$$A_{i,j} = \frac{\partial^2 U}{\partial\alpha_i\partial\alpha_j}, \tag{4}$$

where $\alpha_i = x_{(i+1)/2}$ when i is odd and $\alpha_i = y_{i/2}$ when i is even. Here we suppose the atoms are vibrating only in the plane of the ring with coordinates (x,y). The left (right) self energy is given by [15]

$$\Sigma_{L(R)} = C_s\exp(\imath\theta_{L(R)}), \tag{5}$$

where according to dispersion relation of a mass-spring simple chain, $\theta_{L(R)}$ is

$$\cos\theta_{L(R)} = 1 - \omega^2/2\omega_0^2$$

in which $\omega_0 = \sqrt{C_s/m}$. At the end, the total phonon density of states and transmission coefficient, respectively, are written as

$$\mathrm{DOS}(\omega) = -\frac{2\omega}{\pi N}\sum_{i=1}^{N}\mathrm{Im}\,G_{i,i}(\omega), \tag{6}$$

and

$$T(\omega) = 4\,\mathrm{Im}\,\Sigma_L\,\mathrm{Im}\,\Sigma_R\,|G_{1,2nf-1}|^2. \tag{7}$$

We mention here that if one of the masses in the ring is replaced by a mass $m+\delta m$, then $m\omega^2$ should be changed to $(1+\eta)m\omega^2$ at the corresponding element of G^{-1} in Eq. (3) where $\eta = \delta m/m$. The above formalism enables us to evaluate the phonon transmission coefficient through an atomic ring for some different situations. We will examine numerically this scenario for a benzene-like mass-spring ring in the following cases: (i) the corresponding springs of the single and double bands can be different, (ii) the position of connection atom of the ring with output lead can be changed (iii) one of the masses in the ring will be massive with respect to others.

3. Numerical results for a hexagonal ring

In this section, as a test case, we study the phonon transport properties of a hexagonal mass-spring ring which is enclosed by two simple phononic leads (Fig. 1). In our calculations, we take all the masses in the leads the same and preferably similar to masses of the ring. We also assume all the spring constants in the leads and contacts are identical and equal to $C_s = 1$.