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Heat Conduction Properties of DNA

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Abstract
Thermal conductivity properties of DNA is studied in a lattice of real sequence through PB model developed for DNA dynamic investigations attached to Nose Hoover heat bathes in two ends. Using a chain of real DNA we showed that with introducing a temperature gradient between two end of molecule, DNA can conduct heat flux preferred in a one direction while in the opposite direction DNA act as an insulator. This is what named as thermal rectifier. Rectifier efficiency obtained in this simulation was about 3.

Recently, considering the heat flow process in Nano devices has a great importance due to application in future technology like electronic technology, new energy sources and energy harvesting. This new era in control and manipulate heat flow (phononic) has stimulated much attention to study heat conduction properties in various nano scale devices from materials to molecules.
Some devices to manage and control the heat flow such as thermal rectifier has been proposed. Strictly speaking, thermal rectifier is a device that conducts heat in one direction and prevent in opposite direction. First Terranno et.al showed that to control the heat flux through the chain, one can act on a central part of the system. Also with constant temperature bias, it is attainable to tune the heat flux by altering the temperatures of both thermostats. It was a first time that the possibility of thermal rectifier is approved [1]. Their model is based on PB model that describes DNA dynamic. Nevertheless their parameters aren't real parameters associated to DNA. Afterwards rectification in various models and materials [2-10] experimentally and theoretically were studied. In this paper we show how a sequence of DNA with real parameters can act as a thermal rectifier. We consider the Hamiltonian (1) introduced by Peyrard-Bishop in1989 [11]:

$$H = \sum_{n=1}^{N} \frac{p_n^2}{2m} + V_n(y_n) + \frac{1}{2}k(y_n - y_{n-1}) \qquad (1)$$

In which $V_n(y_n)$ is an onsite potential named as Morse potential (2) and equals to:

$$V_n(y_n) = D_n(e^{-\alpha_n y_n} - 1)^2 \qquad . \qquad (2)$$

Where m is the reduced mass of a base pair, y_n denotes the stretching from equilibrium position of the hydrogen bonds connecting the two bases of the n-th pair and p_n is its momentum.The equations of motion (3) are written follows:

$$m\ddot{y}_n = k(y_{n-1} - 2y_n + y_{n+1}) + 2D_n\alpha(e^{-\alpha_n y_n})(e^{-\alpha_n y_n} - 1) - m\zeta_R u_n \qquad n = 1{:}16$$

$$m\ddot{y}_n = k(y_{n-1} - 2y_n + y_{n+1}) + 2D_n\alpha(e^{-\alpha_n y_n})(e^{-\alpha_n y_n} - 1)$$

$m\ddot{y}_n = k(y_{n-1} - 2y_n + y_{n+1}) + 2D_n\alpha(e^{-\alpha_n y_n})(e^{-\alpha_n y_n} - 1) - m\zeta_L u_n$

(3)

$n = N - 15: N$

$\dot{\zeta}_R = \frac{1}{M}(\sum_{n=1}^{16} mu_n^2 - 16k_B T_R)$

$$\dot{\zeta}_L = \frac{1}{M}(\sum_{n=N-15}^{N} mu_n^2 - 16k_B T_L)$$

In this paper we consider the out-of-equilibrium properties of model (1) by numerically simulating the dynamics of the N particle chain, coupled, at the two ends, with thermal baths at different temperatures T_1 and T_2.We thermalize at T_1 and T_2 the first and the last 16 particles by using Nos´e-Hoover thermostats chains[12]. We compute the local temperature (4) at site n by

$T = \frac{m}{k_B}\langle \dot{y}_n^2 \rangle$

(4)

And the local heat flux (5) using:

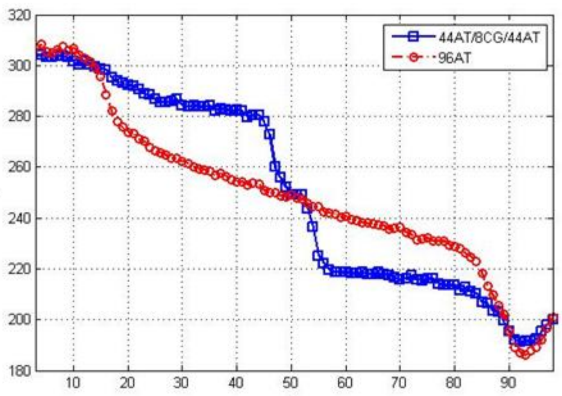
$J_n = k\langle \dot{y}_n(y_n - y_{n-1})\rangle$. (5)

$D_n = 0.075$ At the steady state the local flux is the same at everywhere. As the first step we consider a homogeneous chain composed of 96 AT base pair with parameters $D_n = 0.05\ ev, \alpha_n = 1\ \frac{ev}{\AA}, k = 0.06\frac{ev}{\AA^2}$ for n=1,…,N[11,13]. The sequence is attached in two ends to Nose Hoover heat bath with temperatures T_L and T_R respectively equal to 300 and 200 k. The result showed that ther was a temprature gradient and smooth heat current in the chain(fig1,circles). At the second step if we import an inhomogeneity in the chain with introducing 8 CG base paire in the middle of the chain with , we detect a central insulator part in the chain that avoid flowing the heat flux from right to left as showen in fig1 with rectangels. In another configuration, if we change the right and left thermosates with each other we can see the value of heat flux would change significantly by the factor of 3 which is called as rectifier efficiency, defined as a ratio of forward heat flux to the backward heat flux:

$$\gamma = \frac{J_+}{J_-}$$

. (6)

we measured $J_+ = 10^{-5}$ and the $J_- = 3 \times 10^{-6}$,



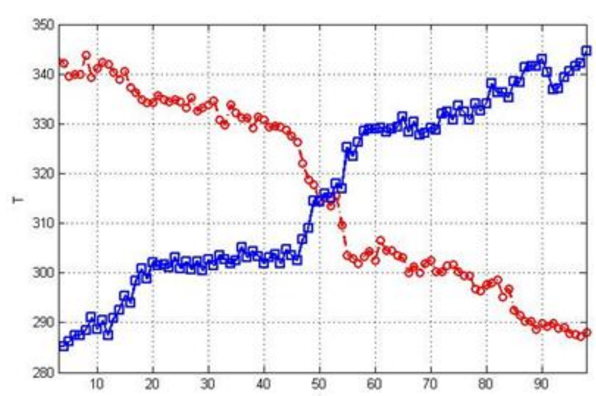


Fig 1: Temperature profile for a homogeneouos chain (red dashed dotted circels) and for nonhomogeneous sequence (blue solid rectangles)

Fig 2: Thermal rectifier for two opposite orientations of the thermal gradient in the nonhomogeneous chain.

Results

The issue of energy transport in low dimensional systems has attracted many interests. Controlling the energy flow in biomolecules is important, for instance when the energy of ATP hydrolysis is released locally in a molecular motor to be used elsewhere after some delay.
In this study we investigate heat conduction properties of DNA sequences attached to Nose Hoover thermostats in two ends. We have showed that homogeneous DNA could show temperature gradient at two ends but If we consider a nonhomogeneous chain, we find that heat flux could not be easily flow through DNA and central part act like insulator and flowing heat flux.
At the next step we design the thermal rectifier.we reverse the direction of thermal gradient and we detect the forward and the backward flux differ by the factor 3.
We will attempt to modify this factor by changing the control parameters of the system such as temperature gradient, thermostat coupling parameters, and the length of nonhomogeneity and so on. and to investigate the role of other parameters in modifying rectifier efficiency.

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