# DNA Nano Wire as a Heat Pump

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## Abstract

*Recently, thermal management in nanoscale devices has been attracted many interests due to desire to attain new sources of energy and on-chip cooling. In this paper, we aim to investigate the effect of periodic external force on the heat flow control in DNA nano wire. It was found that by applying driven force, pumping effect has been observed in DNA. In this way, DNA act as a cooling nano device. The resonance frequencies of DNA have been detected. Threshold amplitude of driving force for attaining permanent pumping effect has been identified. Also, despite of zero temperature bias, there is a directed net heat flow across the chain in driven state.*

…..The issue of energy transport in low dimensional nano systems has attracted many interests [1,2] due to applications such as new source of energy, energy harvesting building, thermal computers[3], thermal logic gates [4], thermoelectric waste heat recovery, and quantum information and so on. In molecular electronics, local heating of nanoscale devices might cause structural instabilities undermining the junction integrity [5]. Engineering good thermal contacts and cooling of the nano junction are necessary for a stable operation of nano mechanical devices, e.g. refrigerators and pumps [6].

During the years after the first report on heat control [7], researchers have been tried to achieve the better control and manipulation of phonons. In this respect, some ingredients of thermal circuit such as thermal diode, thermal transistor and heat pump have been proposed theoretically and to some extent verified experimentally [8]. In spite of relevant progresses, several problems remain open and we are still far from a complete understanding.

In this paper we study heat conduction through DNA nano wire by applying a periodic external force at one end. Control of heat flow through molecules by employing nonlinear interactions might be useful for cooling devices and heat flow controllers in biotechnology.

DNA is a double strand molecule and each strand is a polymeric collection of nucleotides. The nucleotides belonging to the same strand are connected by strong covalent bonds, modeled by the nearest-neighbour anharmonic interactions, while the strands are coupled to each other through the weak hydrogen bonds, modeled by an on-site potential which is nonlinear. In this study, we use PBD model introduced in 1993 by Peyrard Bishop Dauxios[9]. The Hamiltonian of the system is written according to PBD model as follow:

$$H = \sum_{n=1}^{N}\left(\frac{p_n^2}{2m} + V(y_n) + W(y_n, y_{n-1})\right) \qquad (1)$$

Wherein $V(y_n) = D_n(e^{-ay_n} - 1)^2$ is the Morse potential describes the interaction between complementary base pairs and $W(y_n, y_{n-1}) = \frac{k}{2}\left(1 + \rho e^{-b(y_n + y_{n-1})}\right)(y_n - y_{n-1})^2$ specifies the stacking interactions in each strand. Equation of motion for the chain coupled at the two ends with thermal baths at different temperatures is written as:

$$\ddot{y}_n = \frac{2aD_n}{m}(e^{-ay_n})(e^{-ay_n} - 1) - \frac{k}{m}\left(1 + \rho e^{-b(y_n + y_{n-1})}\right)(y_n - y_{n-1}) + \frac{k}{m}\left(1 + \rho e^{-b(y_{n+1} + y_n)}\right)(y_{n+1} - y_n) + \frac{kb\rho}{2m}e^{-b(y_n + y_{n-1})}(y_n - y_{n-1})^2 + \frac{kb\rho}{2m}e^{-b(y_{n+1} + y_n)}(y_{n+1} - y_n)^2 - \delta_{n,r}\varepsilon_R\dot{y}_n - \delta_{n,l}\varepsilon_L\dot{y}_n \qquad (2)$$

The parameters of the model are as follows:

$$D_{AT} = 0.05\ ev, \qquad D_{CG} = 0.075\ ev, a = 1\ {}^{ev}/_{A}\ k = 0.25\ \frac{ev}{\dot{A}^2}, \qquad b = 0.35\ \frac{1}{\dot{A}}, \qquad \rho = 0.5$$

Where r corresponds to 8 right base pairs and l corresponds to 8 left ones. Thermal baths is simulated by Nose Hoover thermostats according to:

$$\dot{\varepsilon}_L = \frac{1}{M}\left[\sum_{n=1}^{8} \frac{p_n^2}{m} - 8k_B T_L\right],\ \dot{\varepsilon}_R = \frac{1}{M}\left[\sum_{n=N-8}^{N} \frac{p_n^2}{m} - 8k_B T_R\right] \tag{3}$$

In which M is the coupling between DNA and reservoirs, $k_B$ is the Boltzmann constant and $T_L, T_R$ are the temperature of the left and right thermostats respectively. Using Virial theorem, we compute the local temperature at site n by: $T = \frac{m}{k_B}\langle \dot{y}_n^2\rangle$ and continuity equation for the energy density implies the local heat flux could be written as:

$$j = -k\left\langle \dot{y}_n \left(\left(1 + \rho e^{-b(y_n + y_{n+1})}\right)(y_{n+1} - y_n) + \frac{\rho b}{2} e^{-b(y_n + y_{n+1})}(y_{n+1} - y_n)^2\right)\right\rangle \tag{4}$$

It is interesting the effect of periodic boundary conditions acted on one end of DNA such as driving forces, time dependent temperature modulation and so on. A time periodic sinusoidal force is applied on the first particle of the DNA sequence. The Hamiltonian of the system is written as $H = H_{PBD} + H_{ext}$ and $H_{ext} = -\delta_{1,n} x_n F_0 \sin(\omega t)$, where, $F_0$ is the amplitude of driving force and $\omega$ is its frequency. $\delta_{1,n}$ implies that the external force imposes to the first base pair. Now, the heat flux as a function of frequency, amplitude and $\Delta T$ has been calculated.

As a first step, by acting the ac driving force on the first particle, heat flux as a function of driving frequency has been calculated. We can see from Fig.1, the heat flux increases at first and then decreases as the driving frequency increases. This behavior means that heat flow has been reversed. On the other words, a heat pumping effect can take place in DNA molecule. Heat pump is a device that provides heat energy from low temperature reservoir to high temperature reservoir, opposite to the direction of spontaneous heat current. In this way, DNA is a cooling device. There exist some values of the driving frequencies at which the heat flux takes its maximum, indicating the resonance frequencies of DNA. It represents the driving frequency is identical with system's oscillation frequencies. So we could identify the internal oscillation frequencies of DNA

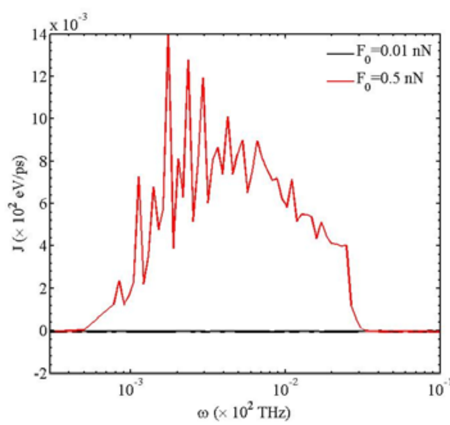
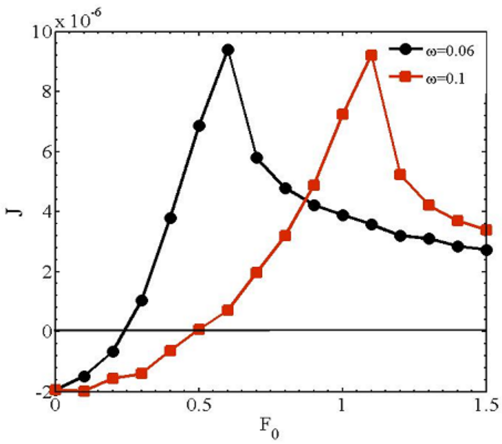



**Fig.1. Heat flux as a function of driving frequencies for various amplitude if sinusoidal force is applied..**

In the following, we consider the dependence of pumping effect on the amplitude of driving force. It was found in moderate frequencies, there is a threshold value for the intensity of external forces which above it, the regime is always

pumping regime. The result has been shown in Fig.2. It is clear in driving frequencies equal to 0.1 and 0.06, threshold amplitude are respectively 0.5 and 0.2. So the smaller threshold is associated to smaller frequencies.

At the next, the dependence of thermal flow to temperature gradient has been investigated for the fixed values of driving frequency and amplitude. Two opposite direction of temperature bias was considered. It was seen that for all temperature biases in the reverse direction, the thermal flow has been reversed. Interestingly, in the zero temperature bias, there is a heat flux in the system. Figure 3 shows the result.



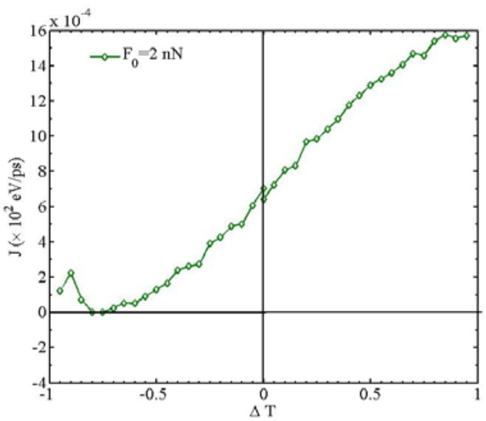




**Fig.3. The pumping effect in terms of temperature bias.**

## Conclusions

Thermal properties of nanowires will become an important factor in the development of upcoming nanoelectronic circuits due to the significance of the thermal control among nanoelements. DNA is one of foremost nanowire materials due to its elastic properties and self-assembly capabilities which make a wide variety of nanostructures possible. We proposed a model of the heat pump, where the heat flux can be directed against the temperature bias by suitably adjusting the frequency of the ac driving force. The dependence of pumping regime on driving frequency, amplitude and temperature bias has been investigated. The resonance frequencies of DNA have been detected. Threshold amplitude for having permanent heat pump was found. Heat control in nano wires has a significance dependence on system parameters. For the exhaustive investigation of this issue, it is important to investigate the effect of some parameters such as system size, sequence combination, temperature region on occurrence of heat pumping phenomenon.

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