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Bifurcation based parameter selection of PBD model in DNA

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Abstract Recently, energy transport in nano-scale devices has been attracted many interests due to desire to achieve new sources of energy and on-chip cooling. Since first report on heat control, many efforts have been done to consider thermal properties of various nano-devices to be used as thermal circuit ingredients. In the recent years, bio-materials such as DNA have been regarded as fascinating nano-wires due to their special mechanical and self-assembly properties. Interestingly, DNA based nano-electronic devices and molecular motors have been constructed. So, considering the heat conduction properties of DNA seems to be important because of utilizing as functional devices. On the other hand, the selection of the potential parameters is a very important issue. In this paper, thermal conduction properties of various sequences based on Peyrard-Bishop- Dauxois model have been investigated. An approach has been proposed for exact tuning of potential parameters of DNA molecule based on Bifurcation analysis.

1 Introduction

Recently it was found that phonons as well as electrons could carry and process information, so the phononics has been emerged as a new field in the engineering and science of phonons [1]. Theoretically, various thermal nano devices have been proposed to manipulate phonon transport such as thermal diode [2], thermal transistor [3], thermal logic gates [4], thermal memory [5] and heat pump [6]. Also, there are some works [7, 8]which experimentally showed the thermal control on nano devices.

In the recent years, bio-materials such as DNA have been regarded as fascinating nano-wires due to their special mechanical and self-assembly properties. Interestingly, DNA based nano-electronic devices and molecular motors have been constructed. So, considering the heat conduction properties of DNA seems to be important because of utilizing as functional devices. To study the heat conduction properties of DNA and its dynamic, it is essential to tune the parameters of models describing DNA. Up now, some schemes have been proposed in parameter selection [9, 10]. In this paper, we will introduce bifurcation based parameter selection scheme. By using new determined parameter, denaturation temperature for two sequences of DNA has been determined. Temperature profile for homogeneous and nonhomogeneous sequences has been plotted.

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2 Model

The most popular model describing DNA introduced by Peyrard Bishop Dauxios in 1993 [11]. In this model DNA regarded as a double stranded chain connected to each other by the nonlinear interactions modeled by Morse potential. In each strand, the interaction between neighboring base pairs is described by an anharmonic potential.
The Hamiltonian of the system described by

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

(y_n) is the Morse potential describing hydrogen bonds between base pairs which is written as follows:
$V(y_n) = D_n(e^{-ay_n} - 1)^2,$
and the stacking interactions was modeled by:

$$W(y_n, y_{n-1}) = \frac{k}{2}\left(1 + \rho e^{-b(y_n + y_{n-1})}\right)(y_n - y_{n-1})^2$$

m is regarded as the reduced mass of a base pair and y_n denotes the stretching

from equilibrium position of the hydrogen bonds connecting the two bases of the nth pair.
To consider the canonical system at the steady state, the whole of system has to be connected to thermal reservoirs at the all nodes. Elapsed time is regarded high enough so the system reaches to steady state. The equilibrium dynamics of the model is investigated by regarding N system nodes connected to thermostats. There are some regular models that have been used to control the temperature as a thermostat include the Anderson thermostat, Berendsen thermostat, Nose-Hoover thermostat, and Langevin thermostat.
Nose and Hoover developed an approach to simulate a deterministic thermostat to overcome the difficulties arising from stochastic processes. Nose-Hoover thermostat consists of only one imaginary variable which simulates system's achieve to favored temperature condition [12].
The equations of motion of the system contacted to heat bath are written as follow:

$$\ddot{y}_n = \frac{2aD_n}{m}(e^{-ay_n})(e^{-ay_n} - 1) - \frac{k}{m}\left[\left(1 + \rho e^{-b(y_n+y_{n-1})}\right)(y_n - y_{n-1}) - \left(1 + \rho e^{-b(y_{n+1}+y_n)}\right)(y_{n+1} - y_n)\right] + \frac{kb\rho}{2m}\left[e^{-b(y_n+y_{n-1})}(y_n - y_{n-1})^2 + e^{-b(y_{n+1}+y_n)}(y_{n+1} - y_n)^2\right] - \xi\dot{y}_n.$$

The dynamic of thermostat is given by:

$$\dot{\xi} = \frac{1}{M}\left[\sum_{n=1}^{8}\frac{p_n^2}{m} - Nk_BT\right].$$

DNA molecule is a double helix and each strand is a polymeric collection of nucleotides. Each nucleotide consists of 3 parts include 5 carbon sugar, nitrogenous base and phosphate group. Nitrogenous bases is divided to four groups. The Adenine, Guanine, Cytosine and Thymine are the mentioned groups. Two chain of nucleotides bond to each other by hydrogen bonds and produce a DNA molecule. The base pairing in CG is stronger than AT base pair because of three hydrogen bonds compared with two hydrogen bonds in AT base pair. So the sequence enriched by CG base pairs is more stable than AT rich one.

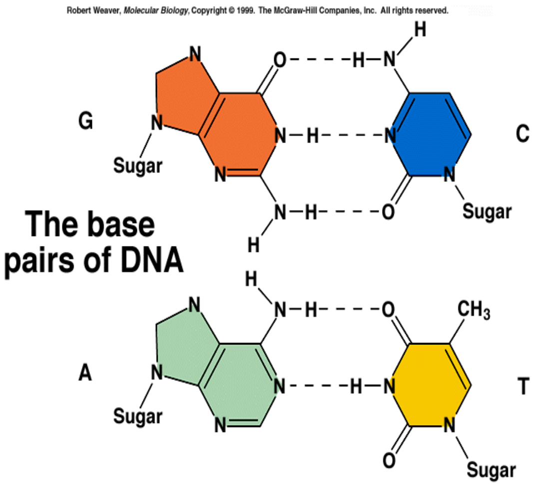

Fig. 1 .The base pairs of DNA

3 Results
3_1 parameter selection

At the first step, we choose two homogenous sequences composed of 32 AT and CG base pairs. The temperature of heat bath is held at 310 k. At the room temperature, the maximum of base pair opening does not exceed more than 1 Angstrom. For a sequence composed of CG base pair, this quantity is decreased by a factor of 1/3. We would like to determine the accurate values of α associated to inverse width of the Morse potential. The system has been allowed to fluctuate. After transient time equal to 10^7 time unit, the bifurcation diagram has been plotted. The results has been shown in Fig. 2(a,b) for AT and CG sequences.

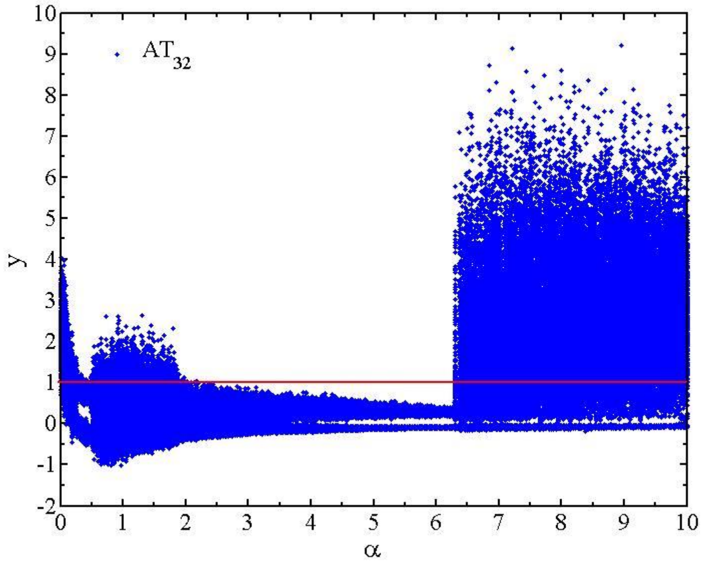

Fig. 2(a). Bifurcation diagram for a sequence composed of 32 AT base pair

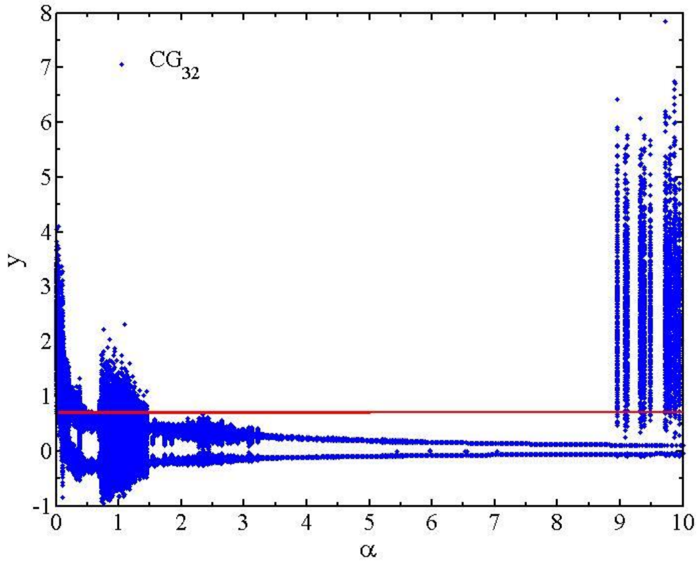

Fig. 2(b). Bifurcation diagram for a sequence composed of 32 AT base pair

The values of α which satisfies maximum fluctuation of DNA have been determined. It has been observed from Fig. 2(a), we can select $\alpha_{AT} = 2\ \dot{A}^{-1}$. While inspired by Fig. 2(b), it has been observed that the best selection for α_{CG} is about $2.4\ \dot{A}^{-1}$.

3_2 Determining Denaturation Temperature

By increasing the temperature of thermal reservoir, the molecule will experience the higher openings. It is known that the base-pairs of a double-helix break up and dissociate from each other to form two separated random coils when a solution of DNA macromolecules is heated up to some crucial temperature. This phenomenon is referred to as DNA denaturation or thermal DNA melting.
With new selected parameters, we investigate the oscillation of base pairs in terms of temperature of heat bath. Figure 3 (a,b) shows the results. It has been obvious that AT sequence undergoes high amplitude openings. At temperatures more the 320k, system will experience thermal denaturation. While for CG sequences, system shows more stable state. In which rare openings has been observed at 350k. So, the DNA needs to more hot reservoir to show phase transition.

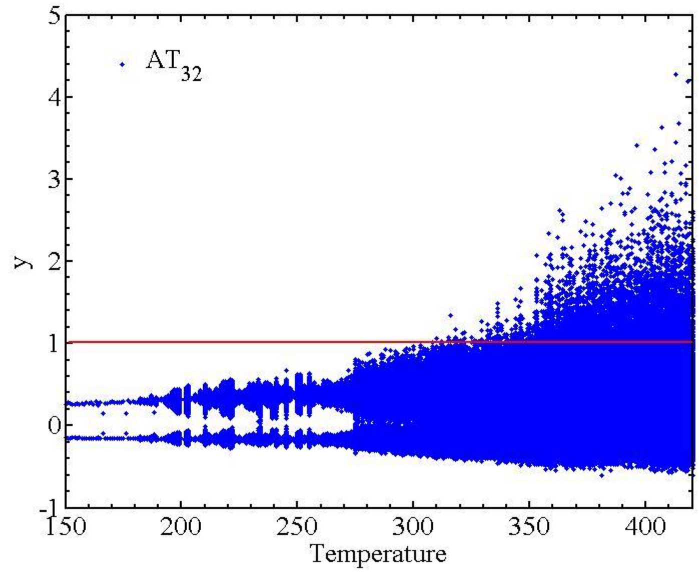

Fig. 3(a). Bifurcation diagram in terms of temperature of heat bath for AT sequence

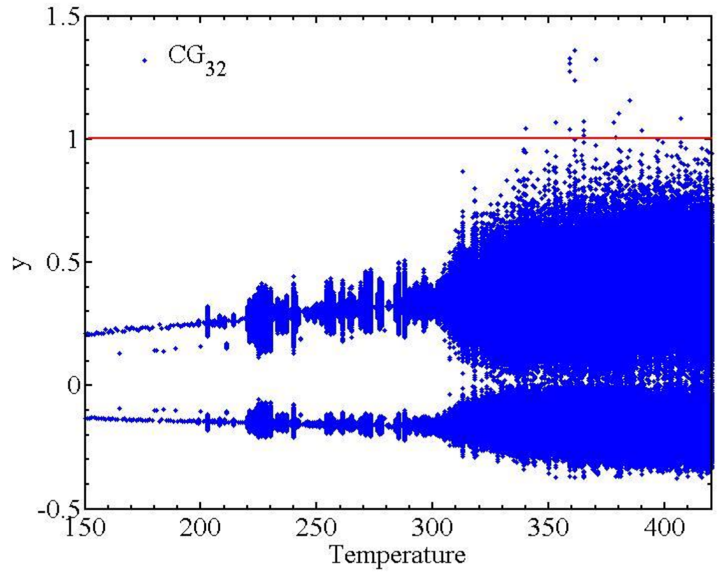

Fig 3(b). Bifurcation diagram in terms of temperature of heat bath for CG sequence

3_3 Heat conduction

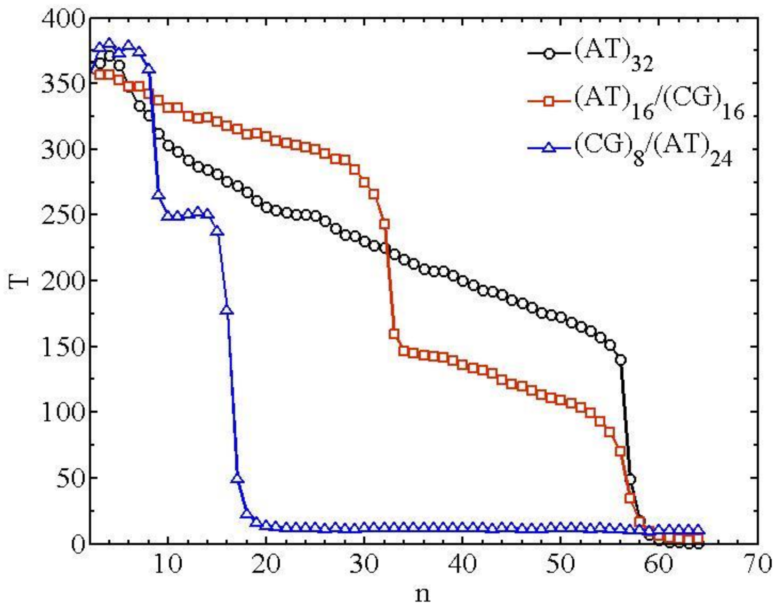

Fig. 4. Temperature profile for homogeneous and nonhomogeneous sequences

Now we investigate heat conduction properties of DNA sequences attached to Nose Hoover thermostats in two ends. We have showed that the homogeneous DNA could show temperature gradient at two ends and smooth temperature profile exhibiting flow of thermal current. But, if we consider some nonhomogeneous chains, we find that heat flux could not be easily flow through DNA and central part act like insulator and prevents flowing heat flux. It could find some application in designing thermal insulating materials and rectification.

4 Conclusion

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. Also, the role of model parameters in investigation of thermal properties of nano wires is crucial.

In this article we suggest a new scenario to determine the value of the one crucial parameter describing DNA dynamics. By using bifurcation diagrams, we could determine the value of invers of width of Morse potential and denaturation temperature for two sequences. As well as, temperature profile for various sequences of DNA has been has been plotted.

References

1. M.Maldovan. Sound and heat revolutions in phononics, Nature, 503 {209, 2013.
2. T. Dauxois, M. Peyrard, and A. R. Bishop. Entropy-driven DNA denaturation. Physical Review E, 47,1 {44, 1993.
3. B. Li, L. Wang, and G. Casati, Negative differential thermal resistance and thermal transistor. Applied Physics Letters, 88, 14 {143501, 2006.
4. L. Wang, and B. Li. Thermal Logic Gates: Computation with phonons. Physical review letters, 99, 17. {177208, 2007.
5. Lei. Wang, and Baowen Li. Thermal memory: a storage of phononic information. Physical review letters, 101, 26 {267203, 2008.
6. D. Segal, and A. Nitzan. Molecular heat pump. Physical Review E, 73, 2, {026109, 2006.
7. W. Kobayashi, Y. Teraoka, and I. Terasaki, An oxide thermal rectifier, Applied Physics Letters. 95, 17, {171905, 2009
8. H. Tian, D. Xie, Y. Yang, T. L. Ren, G. Zhang, Y. F. Wang, ... , L. T. Liu, A Novel Solid-State Thermal Rectifier Based On Reduced Graphene Oxide, Scientific reports, 2, {2012.
9. S. Behnia, et al. A novel approach for the potential parameters selection of Peyrard–Bishop model. Physics Letters A, **375**,7 {1092, 2011.
10. S. Zdravković, and M. V. Satarić. Parameter selection in a Peyrard–Bishop–Dauxois model for DNA dynamics, Physics Letters A, 373, 31 {2739, 2009.
11. T. Dauxois, M. Peyrard, and A. R. Bishop. Entropy driven DNA denaturation, Physical Review E **47**, {684, 1993.
12. W. G. Hoover. Canonical dynamics: equilibrium phase-space distributions, Physical Review A, 31, 3, {1695, 1985.