

Abstract for GR-TR Conference on Statistical Mechanics and Dynamical Systems

Talk Invited

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Statistical and dynamical properties of nonlinear base-pair openings in DNA

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Statistical and dynamical properties of base-pair openings (bubbles) in double stranded DNA will be discussed using the Peyrard-Bishop-Dauxois (PBD) nonlinear dynamical model [1]. A number of successful comparisons with experiments related to base-pair openings will be presented [1, 2, 3, 4].

Theoretical predictions for the position of large thermal openings are compared with experimental results in gene promoter DNA sequences and the most favorable openings occur at transcriptionally relevant sites [5, 6].

Several physical properties of the model will be discussed, like temperature dependent signatures of big bubbles identified in the dynamic structure factor [7], non-exponential decay of base-pair opening fluctuations [8], and the probability distribution of bubble lengths [9].

Finally the structural PBD model will be coupled with a charge propagating along the DNA double helix [10]. Static polaronic solutions and their normal modes related to AC response [11], as well as dynamical charge trapping affecting macroscopic transport parameters [12] will be presented.

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- [1] T. Dauxois, M. Peyrard, and A.R. Bishop, *Phys. Rev. E* **47**, 44 (1993).
 - [2] D. Cule and T. Hwa, *Phys. Rev. Lett.* **79**, 2375 (1997).
 - [3] A. Campa and A. Giansanti, *Phys. Rev. E* **58**, 3585 (1998).
 - [4] S. Ares, N.K. Voulgarakis, K.Ø. Rasmussen, and A.R. Bishop, *Phys. Rev. Lett.* **94**, 035504 (2005).
 - [5] C.H. Choi, et al., *Nucleic Acids Res.* **32**, 1584 (2004).
 - [6] G. Kalosakas, et al., *Europhys. Lett.* **68**, 127 (2004).
 - [7] N.K. Voulgarakis, G. Kalosakas, K.Ø. Rasmussen, and A.R. Bishop, *Nano Lett.* **4**, 629 (2004).
 - [8] G. Kalosakas, K.Ø. Rasmussen, and A.R. Bishop, *Chem. Phys. Lett.* **432**, 291 (2006).
 - [9] S. Ares and G. Kalosakas, *Nano Lett.* **7**, 307 (2007); S. Ares and G. Kalosakas, preprint.
 - [10] S. Komineas, G. Kalosakas, and A.R. Bishop, *Phys. Rev. E* **65**, 061905 (2002); G. Kalosakas, K.Ø. Rasmussen, and A.R. Bishop, *J. Chem. Phys.* **118**, 3731 (2003).
 - [11] P. Maniadis, G. Kalosakas, K.Ø. Rasmussen, and A.R. Bishop, *Phys. Rev. E* **72**, 021912 (2005).
 - [12] G. Kalosakas, K.L. Ngai, and S. Flach, *Phys. Rev. E* **71**, 061901 (2005).