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Talk Invited Invited Talk

Melting of genomic DNA sequences: predictive modeling by nonlinear lattice dynamics

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Over the last twenty years, mesoscopic, nonlinear dynamics-based (Peyrard-Bishop-Dauxois, PBD) modeling has been instrumental in elucidating important qualitative aspects of the cooperative behavior which characterizes the thermal separation of the two DNA strands. Highlights to date include (i) establishing the infinite homopolymer DNA chain as one of the few nonpathological one-dimensional systems which exhibit a true thermodynamic phase transition, (ii) statistical and dynamical modeling of the denaturation bubble involved in the transcription process. Curiously, although this type of minimal, mesoscopic approach is uniquely suited to describe the details of the multistep, cooperative melting process taking place at long genomic sequences, the PBD model has not yet been subjected to this obvious, detailed reality test.

I will present a PBD-based analysis of experimental melting profiles for a number of specific sequences with many thousands of base pairs. The results [1] suggest that it is possible to predict complex melting profiles of long genomic sequences without any adjustable parameters, using only the salt concentration and the sequence data.

The proposed new parametrization of the PBD model - largely based on physically motivated estimates - provides a quantitative understanding of a number of further aspects of DNA structure and/or low-frequency dynamics. Thus, (I) calculated probabilities for single base-pair opening are consistent with the very low values (of the order of 1ppm) obtained from imino proton exchange experiments [2], although (II) extended bubbles may occur with relatively high probabilities at selected sites of genomic sequences, (III) low-frequency transverse optical phonons in model heterogeneous chains are in the range experimentally observed in DNA Raman spectra [3], and (IV) calculated structure factors are in agreement with recent neutron diffraction measurements [4].

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[1] N. Theodorakopoulos, to be published

[2] M. Gueron, M. Kochoyan, J-L Leroy, Nature **328**, 89 (1987).

[3] H. Urabe, Y. Tominaga and K. Kubota, J. Chem. Phys. **78**, 5937 (1983).

[4] A. Wildes, N. Theodorakopoulos, J.Valle-Orero, S. Cuesta-López, J-L Garden and M. Peyrard (to be published).