AKB 6 DNA Mechanics

Time: Monday 14:30–16:00 Room: ZEU 260

AKB 6.1 Mon 14:30 ZEU 260

Bubble Nucleation and Cooperativity in DNA Melting — •Saul Ares[1], Nikolaos K. Voulgarakis[2], Kim Ø. Rasmussen[3], and Alan R. Bishop[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — [2]Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [3]Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The onset of intermediate states (denaturation bubbles) and their role during the melting transition of DNA are studied using the Peyrard-Bishop-Dauxois model by Monte Carlo simulations with no adjustable parameters. Comparison is made with previously published experimental results that used a novel bubble quenching technique based in the possibility of hairpin formation on single strands of DNA. An excellent agreement is found between our theoretical predictions and experimental results. Melting curves, critical DNA segment length for stability of bubbles, and the possibility of a two-state transition are studied. The content of this contribution is published in Physical Review Letters 94, 035504 (2005).

AKB 6.2 Mon 14:45 ZEU 260

An Intermediate Phase in DNA Melting — •Richard A. Neher and Ulrich Gerland — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoSciene (CeNS), LMU München

We predict a novel temperature-driven phase transition of DNA below the melting transition. The additional, intermediate phase exists for repetitive sequences, when the two strands have different lengths. In this phase, the longer strand is completely absorbed onto the shorter strand. The excess bases form mobile bulge loops inside the helical region. Below the transition temperature, more and more of these bulge loops condense into overhanging single stranded ends. We calculate the partition sum of such DNA exactly and find, that this transition is continuous and in many aspects analogous to Bose-Einstein condensation. When the periodicity of the sequence is destroyed by rare point mutations, the transition becomes discontinous. Furthermore, we find that the order of the melting transition of repetitive DNA differs from that of ordinary DNA.

[1] R.A. Neher and U. Gerland, `qbio.BM/0509015`

AKB 6.3 Mon 15:00 ZEU 260

Tracking of Type I restriction enzymes along DNA — •Ralf Seidel[1,2], Joost G. P. Bloom[1], Carsten van der Scheer[1], Nynke H. Dekker[1], Mark D. Szczelkun[3], and Cees Dekker[1] — [1]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — [2]Biotechnolgisches Zentrum, TU Dresden, Germany — [3]Department of Biochemistry, University of Bristol, UK

Type I restriction enzymes are complex cellular machines that cleave foreign, viral DNA using two DNA translocating motor subunits. During the translocation process the core unit of the enzyme complex stays bound to the DNA whilst the motors translocate adjacent DNA and thus pull it towards the enzyme, which results in the formation of large DNA loops. Using magnetic tweezers, we investigated on the level of a single enzyme how the DNA motors track along their DNA template. We found that the motor subunits follow directly the helical pitch of the DNA. Due to the attachment of the motors to the core unit of the enzyme, their rotation around the DNA is inhibited and torsional stress is not released. In this way the DNA gets threaded through the enzyme complex leading to an almost complete untwisting of the DNA in the extruding loop and strongly positively supercoiled DNA in front of the motor. Probing both the translocated distance on the DNA and the amount of generated supercoils, we found that the enzyme translocates 11 ± 2 bp per generated supercoil, which strongly suggests tracking of the DNA helical pitch. We furthermore found that the motors track along the 3'-5' strand by investigating how small single strand gaps are overcome.

AKB 6.4 Mon 15:15 ZEU 260

The effect of semiflexibility on the dynamics of DNA in nucleosomes — •Wolfram Möbius, Richard A. Neher, and Ulrich Gerland — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for Nanoscience (CeNS), LMU München

Even though the DNA in eukaryotic cells is tightly packed with the help of histones, it must be accessible for passively binding regulatory proteins. According to the *site exposure mechanism* [1], these proteins can temporarily gain access to a buried DNA site during conformational fluctuations of nucleosomes, the fundamental packing units consisting of about 150 base pairs of DNA wrapped around a histone complex. Recently, the dynamics of spontaneous partial DNA unwrapping was observed directly, using optical single molecule techniques [2,3]. Here, we study this dynamics within a mesoscopic model of the nucleosome, using Brownian dynamics simulations and theoretical analysis of simplified toy models. We find that the internal polymer dynamics of the semiflexible DNA has a strong impact on the dynamics of our nucleosome model. We characterize this effect in detail and discuss a number of experimentally relevant predictions of our model.

[1] Polach and Widom, Journal of Molecular Biology **254**, 130 (1995)
[2] Li *et al.*, Nature Structural & Molecular Biology **12**, 46 (2005)
[3] Tomschik *et al.*, PNAS **102**, 3278 (2005)

AKB 6.5 Mon 15:30 ZEU 260

Electrostatic interactions of DNA can quantize azimuthal orientations of nucleosome core particles in bilayers — •Andrey Cherstvy and Ralf Everaers — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

We propose that DNA charge distribution can affect electrostatic interactions of nucleosome core particles (NCP) in bilayers and crystals. The bilayers of NCPs are formed by densely packed columns of NCPs, stacked on top of each other with axes nearly parallel to columnar axis. We suggest that mutual azimuthal orientations of NCPs in neighboring columns across the NCP bilayer are quantized with the angle of about 45 degrees. The reason for that is the helical symmetry of DNA charge distribution, with its phosphates and cations adsorbed in the grooves. This results in azimuthal charge "oscillations" on outer circumference of NCPs, along a "ring" of wrapped DNA. When two NCPs are close to each other, these charge patterns can establish an electrostatic zipper, similarly as for two parallel DNA molecules [1]. Our predictions can be tested experimentally, provided a better statistics and resolution of cryoelectron micrographs [2] will be achieved. This can provide new information about inter-nucleosomal electrostatic interactions that influence DNA compactification in chromatin fibers, the phenomenon which is still poorly understood. [1] A. G. Cherstvy, A. A. Kornyshev, and S. Leikin, J. Phys. Chem. B, 106, 13362 (2002); ibid., 108, 6508 (2004) and references therein [2] A. Leforestier, J. Dubochet, and F. Livolant, Biophys. J., 81 2414 (2001).

AKB 6.6 Mon 15:45 ZEU 260

Single Molecule FRET detects sequence dependent Bending and Kinks in DNA — •Filipp Oesterhelt — Heinrich Heine Universität Düsseldorf, Universitätsstrasse 1, Geb. 26.32.02.30, 40225 Düsseldorf

Fluorescence Resonance Energy Transfer (FRET) is a universal tool to measure distances in the range of a few nanometers. This makes FRET ideally suited to analyse distances and distance changes between and within single biomolecules. In the principle accuracy in distance changes is in the sub nanometer range. But the calculation of absolute distances is difficult due to systematic errors. We applied the method of Multiparameter Fluorescence Detection to single DNA doublestrands, internally labelled with a donor and an acceptor fluorophore at various positions. The comparison of the measured energy transfer efficiencies with the fluorophore positions modelled by molecular dynamic simulations revealed that the fluorophore positional and orientational variability has to be taken into account. The absolute distances calculated from our FRET measurements did not only show the helicity of the DNA duplex, but also a sequence dependent bending which was in good agreement with values calculated earlier by NMR and other techniques. We also applied our high precision FRET measurements to the analysis of kinked DNA containing adenosine bulges. From our data we could reconstruct the 3D structure of the kink, revealing the angle, the relative rotation of the helical arms and the offset between their helix axes.