

## DY 40: Statistical Physics of Biological Systems II (joint session DY/BP)

Time: Wednesday 15:00–16:30

Location: ZEU/0114

### Invited Talk

DY 40.1 Wed 15:00 ZEU/0114

#### Learning the statistical folding of bacterial chromosomes —

•CHASE BROEDERSZ — Vrije Universiteit, Amsterdam, Netherlands

The physical organization of bacterial chromosomes is inherently variable, with large conformational fluctuations both from cell to cell and over time. Yet, chromosomes must also be structured to facilitate processes such as transcription, replication, and segregation. A physical description of this dynamic statistical folding of bacterial chromosomes remains largely elusive. Hi-C experiments probe chromosome organization by measuring average contact frequencies of chromosomal loci pairs. I will present a principled approach to infer and analyze the dynamic and statistical organization of chromosomes. In particular, we developed a rigorous and fully data-driven 4D Maximum Entropy approach to extract a generative model for the dynamic organization of a replicating bacterial chromosome directly from time-course Hi-C and microscopy data. This data-driven approach aims to unravel the dynamic statistical folding of chromosomes - and its impact on functional processes - in growing and replicating bacteria. Finally, I will discuss how these data-driven inferences can be used to develop mechanistic insights into the contributions of various chromosome segregation mechanisms, including ParABS and loop-extruding SMC complexes. Together, our results illustrate how changes in the geometry and topology of the polymer, induced by DNA-replication and loop-extrusion, impact the organization and segregation of bacterial chromosomes.

DY 40.2 Wed 15:30 ZEU/0114

#### A freely jointed chain with two-state hinges —

•MINSU YI and PANAYOTIS BENETATOS — Department of Physics, Kyungpook National University, Daegu, South Korea

We discuss aspects of the stretching and bending elasticity of a freely jointed chain, where the hinges can be open or closed in a random fashion. This two-state-hinge model captures a specific degree of freedom associated with the local bending stiffness of the polymer, and its variation can be due to internal changes or to the attachment of ligands from the environment. In this presentation, we focus on comparing the effects of two different types of disorder on the hinges: annealed (reversible Freely Jointed Chain, rFJC) or quenched (quenched Freely Jointed Chain, qFJC). It turns out that, as expected, those different types of disorder yield qualitatively different behaviors. For finite-size systems, we obtain a recurrence relation, which allows us to calculate the exact force-extension relation numerically for an arbitrary size of the system for both systems. In the thermodynamic limit, when the contour length is much larger than the persistence length, we obtain an exact expression for the force-extension relation. The difference between the two systems still exists in the thermodynamic limit.

[1] M. Yi, D. Lee and P. Benetatos, *J. Chem. Phys.* 161 (23): 234908 (2024)

[2] M. Yi and P. Benetatos, *J. Stat. Mech.* 073501 (2025)

DY 40.3 Wed 15:45 ZEU/0114

#### Impact of cytosine methylation on the diffusion of charges

along DNA: a quantum perspective —

•MIRKO ROSSINI, DENNIS HERB, PAUL RASCHKE, and JOACHIM ANKERHOLD — Institute for Complex Quantum Systems, University of Ulm, Ulm, Germany

We develop a coarse-grained tight-binding (TB) framework that treats electrons and holes on equal footing. TB parameters, required to characterize the model, are derived from an ab-initio molecular scheme (linear-combination-of-atomicorbitals (LCAO)) that includes all valence orbitals. Simulations address unmethylated vs. methylated CpG-rich and regulatory sequences sensible to DNA methylation, enabling

us to investigate the impact methylation has on the charge diffusion along models of critical relevance in epigenetics and shedding new light on possible undiscovered mechanisms for epigenetic regulation in cells.

Methylation substantially lowers cytosine charge energies ( $\sim 150$  meV) while leaving the opposite guanine nearly unchanged ( $< 20$  meV), thereby introducing site-selective energetic shifts that redesign diffusion pathways. Statistical investigations, such as time-averaged populations and Inverse Participation Ratio (IPR) analyses, show enhanced electron localization at methylated cytosines, contrasted by increased hole delocalization: these dual trends suppress electron-hole co-localization (localization at same sites) and reduce recombination probability, leading to higher trapping times of excess charges along the DNA. Consistently, modelled excitations lifetimes increase upon cytosine methylation.

DY 40.4 Wed 16:00 ZEU/0114

#### Efficient control of $F_1$ molecular motor —

•DEEPAK GUPTA — Institut für Physik und Astronomie, Technische Universität Berlin, Germany

Designing low-dissipation control driving protocols for small-scale systems is an active field of research. In this talk, I will specifically discuss designing efficient driving procedures for a biomolecular motor—the  $F_1$ ATPase. In general, designing such protocols is challenging due to the spatial nonlinearity of the systems and the presence of environmental thermal fluctuations. Nonetheless, a near-equilibrium (linear response) framework is found to apply to a broad class of small-scale systems. We follow this framework to design non-trivial protocols to drive the  $F_1$ 's  $\gamma$ -shaft to synthesize ATP at low-dissipation cost. Our analysis reveals that the designed protocols, based on the linear response approach, dissipate lower energy as compared to the constant velocity driving protocol for a wide range of protocol durations[1]. In the second part of my talk, I will show our recent experimental results on the  $F_1$  ATPase motor, where we compared the dissipation of driving this motor using two experimentally viable protocols: angle clamp and torque clamp. Our experimental results (supported by analytical findings) suggest that angle clamp driving requires less work than that of the torque clamp[2].

[1] *J. Phys. Chem. Lett.* 13 (51), 11844–11849 (2022). [2] *Phys. Rev. Lett.* 135 (14), 148402 (2025).

DY 40.5 Wed 16:15 ZEU/0114

#### Elementary spectrum for the dissonance curve: from biophysics to number theory of musical harmony —

•ALEXANDRE GUILLET — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Musical harmony, as the ancient problem of finding tunings and scales based on the commensurability of sound waves, has been approached by Helmholtz in terms of a dissonance curve in the frequency domain. This model is here recast in an elementary form related to number theory and a thermodynamical formalism for musical intervals and frequency ratios. The idea of the pioneer of biophysics connects with Riemann's zeta function along the critical line, and Minkowski's question mark measure. The former models rational relationships resulting from the acoustics of a harmonic timbre, while the latter models the probability distribution of the neurocognitive effort to assess the commensurability of frequency pairs. The spectrum of the resulting fractal curve predicts the quasi-periods of widely used musical scales, from the pentatonic division of the octave to microtonal ones, thus constituting a biophysical and mathemusical common ground to harmony across musical genres and cultures.