

## DY 27: Statistical Physics II

Time: Tuesday 10:00–11:30

Location: ZEU 118

DY 27.1 Tue 10:00 ZEU 118

**Fractional Diffusion Equation - Derivation and Numerical Approach** — ●PHILIPP ROTH and IGOR M. SOKOLOV — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, D-12489 Berlin

We consider the continuous limit of a lattice continuous time random walk (CTRW) scheme with power-law waiting-time probability density function (WTD) with position-dependent parameters leading to a variable-order time-fractional diffusion equation. Two different situations are discussed, the ones corresponding to abrupt and to continuous changes of the parameters of the WTD. In the first case we derive the matching conditions for the solutions on the border of two subdiffusive media. In the second case we provide the solution for the case of linearly changing exponent in the WTD. We moreover present a numerical method for the solution of such equations based on the Laplace representation and the Laplace inversion using the Gaver-Stehfest algorithm, and compare our analytical solution with numerical results.

DY 27.2 Tue 10:15 ZEU 118

**Kinetic proofreading of epigenetic patterns** — ●BAHAREH KIANI<sup>1</sup>, FABRIZIO OLMEDA<sup>2</sup>, and STEFFEN RULANDS<sup>3</sup> — <sup>1</sup>Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — <sup>2</sup>Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — <sup>3</sup>Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

During early development, the assignment of cellular identities is closely associated with the acquisition of epigenetic marks on the DNA (DNA methylation). Aberrations in the spatial arrangement of these patterns along the sequence of the DNA lead to the death of the embryo and, in adulthood, are one of the hallmarks of cancer. How, despite the limits imposed by thermodynamics, epigenetic information is precisely encoded along the DNA sequence remains to be understood. Here, we show that the paradoxical co-expression of antagonistic players in the DNA methylation machinery provides an ATP-dependent kinetic proof-reading mechanism which enhances specificity and sensitivity of these patterns by orders of magnitude. We characterise the range of possible behaviours and define optimality conditions of such a mechanism. Finally, by drawing on single-cell sequencing experiments we establish the biological significance of proofreading. Our work highlights the importance of collective, non-equilibrium processes in the establishment of epigenetic marks and sheds new lights on the epigenetic regulation of cell fate decisions in early development.

DY 27.3 Tue 10:30 ZEU 118

**Interfaces: A step beyond the elastic approximation** — ●NIRVANA CABALLERO and THIERRY GIAMARCHI — University of Geneva

Diverse systems including ferroic domain walls, cell fronts, or contact lines have been usually described as disordered elastic systems, even when critical hypotheses of the theory are not satisfied. Solving domain walls dynamics and statics beyond the elastic approximation is still a largely open theoretical/analytical problem. In this work, we propose to address it by analyzing a Ginzburg-Landau model, which describes the main dynamics of driven systems and where interfaces with bubbles and overhangs can be studied. We show the connection between the two-dimensional Ginzburg-Landau model and the one-dimensional elastic description for disordered systems and probe the validity of the elastic theory as a function of "defects". We examine observables such as the interface roughness and the structure factor, both

numerically and analytically. Our simulations and calculations, in addition to making contact with experiments, allow to test and provide insight to develop new analytical approaches to this problem.

DY 27.4 Tue 10:45 ZEU 118

**General solution to the one-dimensional connectivity problem** — FABIAN COUPETTE, ●ANDREAS HÄRTEL, and TANJA SCHILLING — Institut of Physics, University of Freiburg, Germany

We present a general method to obtain the connectivity properties of an arbitrary one-dimensional pairwise interacting n-body system in thermal equilibrium. As input, solely the pair density distribution associated to the equilibrium state is required. Accordingly, if exact analytic results exist for the pair density distribution, the pair connectivity can be determined equally exactly. This is illustrated for fully penetrable and impenetrable rods as well as a repulsive  $1/r^2$  nearest-neighbor interaction potential. We also discuss implications of our work for long-ranged interactions, systems in external fields and higher dimensions.

DY 27.5 Tue 11:00 ZEU 118

**Universality of photon counting below a bifurcation threshold** — ●LISA ARNDT and FABIAN HASSLER — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

At a bifurcation point, a small change of a system's parameter causes a qualitative change in the dynamics of the system. This behavior can, for example, be observed in a parametrically driven system or in a laser. In both systems, the driving strength needs to exceed a threshold before classical radiation is produced. We study the photon counting statistics below the instability threshold, where quantum fluctuations enable the emission of photons. Close to the bifurcation point, these fluctuations are determined by the instability threshold. Here, we focus on one-dimensional bifurcations and provide deeper insight into the universal behavior of the photon counting statistics in different physical systems.

DY 27.6 Tue 11:15 ZEU 118

**Pearl-Necklace-Like Local Ordering Drives Polypeptide Collapse** — ●SUMAN MAJUMDER<sup>1</sup>, ULRICH H.E. HANSMANN<sup>2</sup>, and WOLFHARD JANKE<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — <sup>2</sup>Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma 73019, USA

The collapse of the polypeptide backbone is an integral part of protein folding. Using polyglycine as a probe, we explore the nonequilibrium pathways of protein collapse in water. We find that the collapse depends on the competition between hydration effects and intrapeptide interactions. Once intrapeptide van der Waal interactions dominate, the chain collapses along a nonequilibrium pathway characterized by formation of pearl-necklace-like local clusters as intermediates that eventually coagulate into a single globule. By describing this coarsening through the contact probability as a function of distance along the chain, we extract a time-dependent length scale that grows in a linear fashion. The collapse dynamics is characterized by a dynamical critical exponent  $z \approx 0.5$  that is much smaller than the values of  $z = 1 - 2$  reported for nonbiological polymers. This difference in the exponents is explained by the instantaneous formation of intrachain hydrogen bonds and local ordering that may be correlated with the observed fast folding times of proteins.