DY 7: Statistical Physics (General) I

Time: Monday 10:00–12:45 Location: ZEU 160

DY 7.1 Mon 10:00 ZEU 160

Climbing the Jacob's ladder of path integral approaches: quantum effects by classical polymer theory — •Péter Szabó and Alexandre Tkatchenko — University of Luxembourg, 1511 Luxembourg, Luxembourg

Path integral formalism provides an elegant way to evaluate thermal quantum expectation values in the language of classical physics. In ring polymer path integral methods a quantum object is mapped into a classical polymer ring in an extended, high dimensional phase space, where the beads of the polymer are the replicas of the classical system. The equilibrium averages of this polymer give the corresponding thermal properties of the quantum mechanical system.[1]

We have developed a classical polymer theory for imaginary path integrals to get an exact, low dimensional phase space representation of thermal quantum systems. This new picture preserves the classical description, but it allows us to get rid of the curse of dimensionality. The computational complexity of the problem does not depend anymore on the number of replicas. The quantum expectation values can be evaluated by the sampling of the original, classical phase space. The performance of this method is tested in molecular systems, where we calculated the quantum partition functions and compared them to the exact results.

[1] D. Chandler and P. G. Wolynes, J. Chem. Phys. **74**, 4078 (1981)

DY 7.2 Mon 10:15 ZEU 160

The Five Problems of Irreversibility — •Michael te Vrugt — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

Macroscopic thermodynamics has a clear arrow of time: Systems irreversibly approach equilibrium accompanied by a monotonous increase of entropy. This stands in contrast to the laws of microscopic theories, which are invariant under time-reversal. The question how this difference can be explained has created a long debate, with suggestions involving coarse-graining methods as well as cosmological considerations about the entropy of the early universe. In this talk, I will show that a part of the difficulty in solving the problem of irreversibility arises from the fact that it actually consists of five different sub-problems, which are mixed in most discussions. Understanding why these problems have to be distinguished and how they are related to each other then allows to solve them on the basis of modern nonequilibrium statistical mechanics.

DY 7.3 Mon 10:30 ZEU 160

Nonconservative forces and the fluctuation-dissipation theorem — •Kiryl Asheichyk[1,2] and Matthias Krüger[3] — [1]4th Institute for Theoretical Physics, University of Stuttgart, Germany — [2]Max Planck Institute for Intelligent Systems, Germany — [3]Institute for Theoretical Physics, University of Göttingen, Germany

An equilibrium system which is perturbed by an external potential relaxes to a new equilibrium state, a process obeying the fluctuation-dissipation theorem (FDT). In contrast, perturbing by nonconservative forces yields a nonequilibrium steady state, and FDT can in general not be applied. Here we exploit a freedom inherent to linear response theory: Force fields which perform work that does not couple statistically to the considered observable can be added without changing the response. Using this freedom, we demonstrate that FDT can be applied for certain nonconservative forces. In particular, for the case of shear perturbation, this yields a response formula, alternative to and advantageous over the known Green-Kubo relation.

[1] K. Asheichyk and M. Krüger, arXiv:1908.11287.

[2] K. Asheichyk, A. P. Solon, C. M. Rohwer, and M. Krüger, J. Chem. Phys. 150, 144111 (2019).

DY 7.4 Mon 10:45 ZEU 160

Entanglement entropy of random partitioning — •Gergö Roosz[1], Istvan Kovacs[2], and Ferenc Igloi[3] — [1]TU Dresden — [2]Northwestern University, USA — [3]Wigner RCP, Budapest

We study the entanglement entropy of random partitions in one- and two-dimensional critical fermionic systems. In an infinite system we consider a finite, connected (hypercubic) domain of linear extent L, the points of which with probability p belong to the subsystem. The leading contribution to the average entanglement entropy is found to scale with the volume as $a(p)L^D$, where $a(p)$ is a non-universal function, to which there is a logarithmic correction term, $b(p)L^{D-1}\ln L$. In $1D$ the prefactor is given by $b(p)=\frac{c}{3}f(p)$, where c is the central charge of the model and $f(p)$ is a universal function. In $2D$ the prefactor has a different functional form of p below and above the percolation threshold.

DY 7.5 Mon 11:00 ZEU 160

A microscopic model for the computation of dielectric relaxation phenomena in composite systems — •Sujith Reddy Varakantham and Herbert Kliem — Institute of Electrical Engineering Physics, Saarland University, Saarbrücken, Germany

Dielectric relaxation in single phase and composite systems is computed using a microscopic model comprised of thermally activated dipoles fluctuating in double well (DW) potentials. The dipoles interact with each other by their Coulomb forces, thereby influencing mutually the properties of the DWs. To find the time dependent polarization response, a Monte-Carlo simulation method is employed by combining deterministic calculation of potentials with a probabilistic random number. By the interaction, the polarization response changes from Debye to stretched exponential. Afterwards, the time dependent polarization is transformed into the frequency domain. Two single systems with different DW barrier heights, i.e., different relaxation times and also with different distribution of barrier heights are computed first. Then the systems are combined in series connection as well as in embedded systems. While the individual systems exhibit stretched exponential responses with varied stretching factors corresponding to fixed and distributed barrier heights of the DWs, composed systems, on the other hand, show an intermediate behavior comprising both responses. To validate our simulation results, experiments are carried out using a series combination of aluminium and hafnium oxides, each having different dielectric responses. Our simulation results are in agreement with the experimental findings

DY 7.6 Mon 11:15 ZEU 160

Extreme value statistics of ergodic Markov processes from first passage times in the large deviation limit — •David Hartich and Aljaz Godec — Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany

Extreme value functionals of stochastic processes are inverse functionals of the first passage time — a connection that renders their probability distribution functions equivalent. Here, we deepen this link and establish a framework for analyzing extreme value statistics of ergodic reversible Markov processes in confining potentials on the hand of the underlying relaxation eigenspectra. We derive a chain of inequalities, which bounds the long-time asymptotics of first passage densities, and thereby extrema, from above and from below [1]. The bounds involve a time integral of the transition probability density describing the relaxation towards equilibrium. We apply our general results to the analysis of extreme value statistics at long times in the case of Ornstein-Uhlenbeck process and a 3D Brownian motion confined to a sphere, also known as Bessel process. We find that even on time-scales that are shorter than the equilibration time, the large deviation limit characterizing long-time asymptotics can approximate the statistics of extreme values remarkably well. Our findings provide a novel perspective on the study of extrema beyond the established limit theorems for sequences of independent random variables and for asymmetric diffusion processes beyond a constant drift.

[1] D. Hartich and A. Godec, J. Phys. A, 52 (2019) 244001.

15 min. break.

DY 7.7 Mon 11:45 ZEU 160

Microscopic reweighting for non-equilibrium steady states dynamics — •Marius Bause, Timon Wittenstein, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Computer simulations generate trajectories at a single, well-defined thermodynamic state point. Statistical reweighting offers the means to reweight static and dynamical properties to different equilibrium state points by means of analytic relations. We extend these ideas to non-equilibrium steady states by relying on a maximum path entropy formalism subject to physical constraints. Stochastic thermodynamics analytically relates the forward and backward probabilities of any pathway through the external non-conservative force, enabling reweighting both in and out of equilibrium. We avoid the combinatorial explosion of microtrajectories by systematically constructing pathways through Markovian transitions. We further identify a quantity that is invariant to dynamical reweighting, analogous to the density of states in equilibrium reweighting.(M.Bause,T.Wittenstein,K.Kremer,T.Bereau, PRE(in press))

DY 7.8 Mon 12:00 ZEU 160

The quantum first detection problem — •Felix Thiel[1,2], David A. Kessler[2], and Eli Barkai[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany — [2]Department of Physics, Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 52900, Israel

An observer prepares a quantum particle at position x_{in} on a lattice and wants to find its (random) time of arrival T in the target position x_{d}. To avoid complications related to wave function collapse and the quantum Zeno effect, he must adhere to a detection protocol. That means he attempts to detect the particle in the target at the times $\tau, 2\tau, 3\tau, \ldots$, where τ is the detection period, a free parameter. The time T of the first successful detection attempt is the first detection time that generalizes a classical random walker's first-passage time to the quantum realm. Such a situation can easily be implemented in optical quantum walk or waveguide experiments.

In this contribution, we outline the quantum first detection theory and its similarities to first passage theory. We obtain the probability F_n of first detection at the n-th attempt and focus on its asymptotic decay for large times. We present numerical and analytical results for tight-binding quantum walks on one or higher-dimensional simple-cubic lattices.

DY 7.9 Mon 12:15 ZEU 160

Non-Flat Histogram Techniques for Spin Glasses — •Fabio Mueller, Stefan Schnabel, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

We study the bimodal Edwards-Anderson spin glass comparing established methods, namely the multicanonical method, the 1/k-ensemble and parallel tempering, to an approach where the ensemble is modified by simulating power-law-shaped histograms in energy instead of flat histograms as in the standard multicanonical case. We show that by this modification a significant speed-up in terms of mean round-trip times can be achieved for all lattice sizes taken into consideration.

DY 7.10 Mon 12:30 ZEU 160

Asymmetric nascent Dirac delta functions and their application to probability and mechanics — •Jens Christian Claussen — Department of Mathematics, Aston University, Birmingham B4 7ET, U.K.

The Dirac delta distribution is ubiquitious from quantum mechanics and statistical physics to Fourier analysis. In theoretical physics lectures, a commonly presented approach uses a series of nascent delta functions which are normalized and localized and converge point-wise to zero except at the origin. For simplicity, nascent delta functions are usually chosen to be even, i.e. $\delta_n(x) = \delta_n(-x)$. However, this is not a necessary assumption, and in physical interactions as the inelastic collision of two rigid bodies, the force between the particles as a function of time may follow an asymmetric profile; nevertheless with the total momentum transferred in a Dirac delta pulse in the limit of an infinesimal short interaction time.

Here I discuss asymmetric nascent Dirac delta functions and their implications in probability and physics. The gross advantage of asymmetric nascent delta functions is found in their application to probability theory. By introduction of totally asymmetric nascent delta functions, the inconsistencies of using the Dirac delta in mixed discrete-continuous probability spaces when arriving at the cumulative distribution function are resolved. It is anticipated that asymmetric nascent delta functions find further applications in mathematical physics and the theory of measurement.