DY 25: Statistical Physics II (General)

Time: Tuesday 10:00–13:00 Location: BH-N 243

DY 25.1 Tue 10:00 BH-N 243

Analyzing tunneling time distributions on the basis of first passage time problems — •Jeanette Köppe[1], Michael Beyer[1], Markus Patzold[1], Wilfried Grecksch[2], and Wolfgang Paul[1] — [1]Institut für Physik, MLU Halle-Wittenberg — [2]Institut für Mathematik, MLU Halle-Wittenberg

In 1966, E. Nelson established a new interpretation of quantum mechanics, whereby the particles follow some conservative diffusion process, i.e. forward-backward stochastic differential equations (FBSDEs), which are equivalent to the Schrödinger equation. In analogy to classical mechanics, we show that finding the Nash equilibrium for a stochastic optimal control problem, which is the quantum equivalent to Hamilton's principle of least action, a set of quantum dynamical equations can be derived, which are the generalization of Hamilton's equations of motion to the quantum world.

On the basis of these quantum Hamilton equations, it was possible to study tunneling processes in a one-dimensional double-well potential by analyzing first passage times of the respective diffusion processes. We show that the energy splitting between the two lowest energy states $\Delta E = E_1 - E_0$ can be predicted based upon mean first passage times. Moreover, the probability density function of these first passage times is analyzed. The general form of this empircal determined distribution can be motivated by the definition of first passage times and it turns out that, independent of the considered system, tunnel times follow the same distribution qualitatively.

DY 25.2 Tue 10:15 BH-N 243

THE CONCEPT OF TEMPERATURE IN OPEN QUANTUM SYSTEMS: A MICRO-CANONICAL APPROACH — •Camilo Alfonso Moreno Jaimes and Juan Diego Urbina — Institute für Theoretische Physik, Universität Regensburg, Germany

We aim to investigate the concept of temperature in the Open Quantum System (system+reservoir) approach staring from a microcanonical bath scenario where the temperature is not a fundamental but a derived auxiliary concept. When the usual weak coupling regime is assumed, it is well known that the temperature emerges as an effective function of the energy from the saddle-point analysis that justifies the classic ensemble equivalence in the thermodynamic limit[1]. In the strong coupling regime, however, the energy is no longer an extensive quantity and we need a redefinition of temperature. We develop a microscopic analysis based on the Feynmann-Vernon approach to investigate the emergence and meaning of temperature in this strong coupling regime.

[1]: G. Horwitz. Commun. Math. Phys. 89, 11%129 (1983).

DY 25.3 Tue 10:30 BH-N 243

Efficient method of simulating with long-range interactions: The case of coarsening in the Ising model — •Henrik Christiansen, Suman Majumder, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

Simulations of systems with long range interactions are computationally more challenging than its short range counterpart, e.g., in the long range Ising model all spins have to be considered in the calculation of the local energy change. For several models, this problem has been overcome by the introduction of cluster algorithms for equilibrium simulations. As those cluster methods do not capture the dynamics, one cannot rely on them for simulating kinetics of phase transitions. Here, we present a novel and efficient approach of tackling such problems, concerning nonequilibrium dynamics via Monte Carlo simulations by storing a local "pseudo heatbath" for the energy calculation. As an illustration, we present results for coarsening of the long range Ising model in $d = 2$ dimensions. In contradiction to all available simulation results in this context (using an cut-off to make the simulation feasible), our results establish agreement with the theoretical predictions.

DY 25.4 Tue 10:45 BH-N 243

Derivation of an optimal time-dependent bias for Wang-Landau simulations — •Andreas Heuer and Myra Biedermann — Inst. f. Phys. Chemie, WWU Münster, Germany

Among the large variety of free-energy methods, the Wang-Landau approach plays an important role due to its broad applicability, e.g., in the fields of statistical physics. Empirically, it has been observed for simulations of, e.g., the Ising model, that the added bias f(t) should be chosen as M/t for long times, where M denotes the number of bins [1].

In this contribution we analyse a simple but non-trivial model system, suggested in [2], for which the impact of a time-dependent bias can be treated analytically. Key results are: (1) a minimal error requires the choice f(t) = M/t. (2) There exists a short-time regime where the optimum bias decreases exponentially with time. (3) Surprisingly, the estimation of individual free energies is systematically biased, with the bias scaling as log(t) / t.

These results are quantitatively reproduced in simulations of the Ising model and may serve as a justification for a frequently employed application scheme for Wang-Landau simulations, the 1/t algorithm [1].

[1] R.E. Belardinelli and V.D. Pereyra, Phys. Rev. E 75, 046701 (2007). [2] R.E. Belardinelli, V.D. Pereyra, R. Dickman, B. J. Lourenco, J. Stat. Mech., P07007 (2014).

DY 25.5 Tue 11:00 BH-N 243

Interplay of fast and slow degrees of freedom in the disk to slab transition — •Andreas Tröster[1], Clemens Moritz[2], and Christoph Dellago[2] — [1]Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Wien, Austria — [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria

Rare transitions between long-lived stable states are often analyzed in terms of free energy landscapes computed as functions of a few collective variables. Here, using transitions between geometric phases as example, we demonstrate that the effective dynamics of a system along these variables are an essential ingredient in the description of rare events and that the static perspective provided by the free energy alone may be misleading. In particular, we investigate the disk-to-slab transition in the two-dimensional Ising model starting with a calculation of a two-dimensional free energy landscape and the distribution of committor probabilities. While at first sight it appears that the committor is incompatible with the free energy, they can be reconciled with each other using a two-dimensional Smoluchowski equation that combines the free energy landscape with state dependent diffusion coefficients. These results illustrate that dynamical information is not only required to calculate rate constants, but may also be necessary to understand how a given process occurs.

15 min. break

DY 25.6 Tue 11:30 BH-N 243

Irreversible Markov chains in spin models: Topological excitations — •Ze Lei[1] and Werner Krauth[1,2] — [1]Ecole Normale Superieure, Paris, France — [2]The University of Tokyo, Tokyo, Japan

We analyze the convergence of the irreversible event-chain Monte Carlo algorithm for continuous spin models in the presence of topological excitations.

In the two-dimensional XY model, we show that the local nature of the Markov-chain dynamics leads to slow decay of vortex–antivortex correlations in comparision with the fast decorrelation of spin waves.

We propose an assignment algorithm for pairing vortices and antivortices, and show that the maximum vortex–antivortex distance follows a Fréchet description. The contributions of topological excitations to the equilibrium correlations vary from a dynamical critical exponent $z \sim 2$ at the critical temperature to $z \sim 0$ in the limit of zero temperature.

In the harmonic approximation of spin waves for dimensions higher than 2, we confirm the event-chain algorithm's fast relaxation (corresponding to $z = 0$). Its mixing times however remain much larger than equilibrium correlation times at low temperatures.

We also describe the respective influence of topological monopole–antimonopole excitations and of spin waves on the event-chain dynamics in the three-dimensional Heisenberg model.

We expect that the fast relaxation of phonon modes explains the success of the event-chain algorithm at high densities for particle systems.

DY 25.7 Tue 11:45 BH-N 243

Lee-Yang zeros and large-deviation statistics of a molecular zipper — •Aydin Deger, Kay Brandner, and Christian Flindt — Department of Applied Physics, Aalto University, 00076 Aalto, Finland

The complex zeros of partition functions were originally investigated by Lee and Yang to explain the behavior of condensing gases. Since then, Lee-Yang zeros have become a powerful tool to describe phase transitions in interacting systems. Today, Lee-Yang zeros are no longer just a theoretical concept; they have been determined in recent experiments. In one approach, the Lee-Yang zeros are extracted from the high cumulants of thermodynamic observables at finite size [1]. Here, we employ this method to investigate a phase transition in a molecular zipper [2]. From the energy fluctuations in small zippers, we can predict the temperature at which a phase transition occurs in the thermodynamic limit. Even when the system does not undergo a sharp transition, the Lee-Yang zeros carry important information about the large-deviation statistics and its symmetry properties. Our work suggests an interesting duality between fluctuations in small systems and their phase behavior in the thermodynamic limit. These predictions may be tested in future experiments.

[1] K. Brandner, V. F. Maisi, J. P. Pekola, J. P. Garrahan, and C. Flindt, Phys. Rev. Lett. **118**, 180601 (2017)
[2] A. Deger, K. Brandner and C. Flindt, arXiv: 1710.01531 (2017)

DY 25.8 Tue 12:00 BH-N 243

Geometric frustration in non-periodic mechanical metamaterials — •Erdal C. Oğuz[1], Anne Meeussen[2,3], Martin van Hecke[2,3], and Yair Shokef[1] — [1]School of Mechanical Engineering and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel — [2]Huygens-Kamerlingh Onnes Laboratory, Universiteit Leiden, PO Box 9504, 2300 RA Leiden, the Netherlands — [3]AMOLF, Science Park 104, 1098 XG Amsterdam, the Netherlands

We investigate geometric frustration in two-dimensional lattice-based mechanical metamaterials comprised of anisotropic triangular building blocks T, where each such T possesses a nontrivial floppy mode of deformation. When each triangle is oriented randomly neighboring triangles typically cannot deform self-consistently. On the one hand, we analyze the conditions under which a non-periodic packing of these blocks form compatible and frustration-free large-scale structures, i.e., structures that exhibit a global floppy mode that is compatible with the local deformations of each T. By mapping to an antiferromagnetic Ising model, we find an extensive number of possibilities to construct a compatible structure: ($\Omega_0 \sim \exp(T)$). On the other hand, we study incompatible metamaterials in detail and we reveal two distinct types of source of frustration (defects) which either highly localize the frustrated region to a small and finite domain (local defects) or cause delocalized and long-ranged multi-stable conflicts (topological defects) whose multi-stability scales as $\Omega \sim \exp(\sqrt{T})$.

DY 25.9 Tue 12:15 BH-N 243

Explanation of Cosmic Inflation by Phase Transitions — •Hans-Otto Carmesin[1,2,3] and Matthias Carmesin[4] — [1]Universität Bremen, Fachb. 1, Pf. 330440, 28334 Bremen — [2]Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — [3]Gymnasium Athenaeum, Harsefelder Str. 40, 21680 Stade — [4]Universität Göttingen, Fak. f. Physik, 37077 Göttingen

From the Cosmic Microwave Background CMB the flatness problem and the horizon problem arose. An extraordinarily rapid increase of distances in the early universe, the Cosmic Inflation, was proposed as a possible solution (Guth, Phys. Rev. D, 1981), whereby suggested mechanisms for such an increase have been criticized (Steinhardt: Scientific American, 2011). We propose a theory that explains the Cosmic Inflation by a sequence of symmetry breaking phase transitions at critical densities (Carmesin, H.-O.: Vom Big Bang bis heute mit Gravitation - Model for the Dynamics of Space. Berlin: Verlag Dr. Köster, 2017.). Our theory applies first principles only, namely gravitation and quantum physics, contains no fit parameter, applies fundamental constants only, namely the constant of gravitation G, the velocity of light c and the Planck constant h, is in excellent quantitative agreement with observations, namely the critical density, the duration of cosmic inflation, the temperature fluctuations as well as the factor of increase correspond to the CMB and the flatness and horizon problems are solved.

DY 25.10 Tue 12:30 BH-N 243

Clock Monte Carlo: General methods for $O(1)$ complexity — •Manon Michel[1], Xiaojun Tan[2], and Youjin Deng[2] — [1]Centre de Mathématiques Appliquées, UMR 7641, Ecole Polytechnique, France. — [2]Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

Despite a now long history, the most successful and influential Markov-chain Monte Carlo (MCMC) algorithm remains the founding Metropolis algorithm. Sampling the rejection or acceptance of a proposed move requires however estimating the induced global energy change. It can lead to heavy computational overhead when simulating systems with long-range interactions or a large number of coupling terms – e.g. gravitational force, Coulomb force between electric charges, van-der-Waals force, dipole-dipole interaction etc.

Several techniques reduce the complexity but only for specific algorithms and systems. We will present a general technique for constant-time sampling: the "clock" method. We shall explain how this method draws on the factorized Metropolis filter to sample the successive steps of the chain and exhibit its performance for different long-range $O(n)-$spin systems. Besides being simple and powerful, the clock technique is general for a large class of MCMC methods and physical systems, as it relies only on the extensivity of the energy.

DY 25.11 Tue 12:45 BH-N 243

Excited States in Nelson's Stochastic Mechanics — •Markus Patzold[1], Jeanette Köppe[1], Michael Beyer[1], Wilfried Grecksch[2], and Wolfgang Paul[1] — [1]Martin Luther Universität Halle-Wittenberg, Institut für Physik — [2]Martin Luther Universität Halle-Wittenberg, Institut für Mathematik

In 1966 Edward Nelson successfully derived the Schrödinger equation for non-relativistic spinless particles in the ground state using stochastic differential equations (FBSDE). Solutions of the Schrödinger equation can be used to generate particle paths in this context. Pavon generalized his ideas 1995 to the quantum Hamilton principle, similar to the classical one, introducing a stochastic variational principle. Furthermore, a stochastic optimal control approach is equivalent to the above mentioned one and can be solved without the Schrödinger equation as it was shown by Köppe, et al. in 2017.

However, these equations lead to the ground state of the system only. In the talk I will show how to bypass this problem, adapting the stochastic equations, by exploiting the concept of supersymmetry (SUSY) to give iterative equations for all excited states in arbitary dimensions. Numerical calculations for the double well and hydrogen problem as well as analytical calculations for the harmonic oscillator in d dimensions and the radial hydrogen part including a symmetry analysis will be discussed.