# DY 41: Statistical Physics: General

Time: Thursday 9:30–12:45 Location: BH-N 128

DY 41.1 Thu 9:30 BH-N 128

**Survival probability of stochastic processes beyond persistence exponents** — •Maxim Dolgushev — Laboratoire de Physique Théorique de la Matière Condensée, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France

How long does it take a random walker to find a "target"? This time, called the first-passage time (FPT), appears in various domains: time taken by a predator to find its prey or by a transcription factor to find a specific sequence on the DNA, time taken by a virus to infect a cell or by a financial asset to exceed a certain threshold, time taken for the cyclization of a polymeric chain, etc.

From a theoretical point of view, a crucial parameter to evaluate FPTs is the possible presence of a geometrical confinement. For a symmetric random walk in a confined domain, the mean FPT $\langle T \rangle$ is in general finite. The opposite case of unconfined random walks is radically different. In this case, either the walker has a finite probability of never finding the target (transient random walks), or he reaches it with probability one (recurrent random walks) and the probability of survival of the target decreases algebraically with time, $S(t) \sim S_0/t^\theta$.

Our main result is a general exact relation for a process with stationary increments (more generally, for a process whose increments become stationary at long time only), Markovian or not, between the full asymptotic behavior (defined in the absence of confinement) and the mean FPT $\langle T \rangle$ for the same process in a large confinement volume.

DY 41.2 Thu 9:45 BH-N 128

**Perturbative approach to non-linear non-Markovian vibrational spectroscopy** — •Hélène Colinet — AG Netz, FU Berlin

Using perturbation theory, we investigate how non-harmonic potential contributions and non-Markovian friction influence vibrational absorption spectra, in particular the OH stretch band in liquid water. Non-Markovian friction gives rise to homogeneous and inhomogeneous line broadening of vibrational bands and is accurately accounted for using the generalized Langevin equation.

Our analytical results are validated by numerical simulations of the generalized Langevin equation, by which we demonstrate that our perturbation theory successfully reproduces changes in line shape and position. In particular, we show that the non-harmonic bond potential is crucial for resolving the inhomogeneous line broadening of the OH stretch band in the infrared absorption spectrum of liquid water. For this, anharmonic bond potentials and time-dependent friction kernels are extracted from ab initio molecular dynamics simulations.

DY 41.3 Thu 10:00 BH-N 128

**Stochastically driven motion under nonlinear, Coulomb-tanh friction — a basic representation of the consequences of shear thinning** — Theo Lequy[1] and •Andreas M. Menzel[2] — [1]Eidgenössische Technische Hochschule Zürich, Rämistrasse 101, 8092 Zürich, Switzerland — [2]Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Nonlinear friction is abundant in nearly all kinds of scenarios of relative motion. We here consider the stochastically driven dynamics of an object that is subject to the so-called Coulomb-tanh friction force [1]. This force increases linearly with speed at small magnitudes of the velocity and levels off at a constant value at large speeds. In this way, it interpolates between linear and solid (dry, Coulomb) friction. Under such conditions, in the case of one-dimensional motion, we find that the velocity spectrum can be found by formally linking the mathematical description to a Schrödinger equation including a Pöschl-Teller potential. Thus, an analytical approach is possible. We consider the velocity and displacement statistics of individual objects and find intermediate non-Gaussian tails in the spatial distribution function that are pushed outward over time. Both limits of linear and solid (dry, Coulomb) friction are well reproduced. For instance, our description should apply to the case of an object driven on a vibrated substrate covered by a layer of shear-thinning material that leads to the mentioned nonlinear friction.

[1] Theo Lequy, Andreas M. Menzel (submitted).

DY 41.4 Thu 10:15 BH-N 128

**Oscillating autocorrelation functions and their physical implications in equilibrium odd-diffusive systems** — •Erik Kalz[1], Hidde D. Vuijk[2], Jens-Uwe Sommer[3,4,5], Ralf Metzler[1,6], and Abhinav Sharma[2,3] — [1]University of Potsdam, Germany — [2]University of Augsburg, Germany — [3]Leibniz-Institute for Polymer Research, Dresden, Germany — [4]Technical University Dresden, Germany — [5]Technical University Dresden, Cluster of Excellence Physics of Life, Germany — [6]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

Autocorrelation functions (ACF) can be shown to decay monotonically in equilibrium systems. Despite being in equilibrium, this strict monotonicity condition of ACFs is broken in so-called odd-diffusive systems, which are characterized by probability fluxes perpendicular to density gradients. In fact, the velocity-ACF of a tracer-colloid can even be shown to be oscillatory. In normal systems, the monotonic decay of the velocity-ACF translates into an interaction-induced reduction of the diffusion coefficient of the colloid (Green-Kubo relation). We show that in odd systems, the non-monotonicity of the ACF instead results in an enhancement of the tracer diffusion with interparticle interactions.

Ref: E. Kalz, H. Vuijk, J.-U. Sommer, R. Metzler and A. Sharma: Oscillatory force autocorrelations in equilibrium odd-diffusive systems (PRL accepted manuscript)

DY 41.5 Thu 10:30 BH-N 128

**Finite-size excess-entropy scaling for simple liquids** — •Mauricio Sevilla, Atreyee Banerje, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Integral equations in statistical mechanics play a crucial role in connecting thermodynamics to microscopic properties of simple liquids. In computer simulations, these integral equations manifest explicit and implicit size effects that arise from systems with a fixed number of particles and periodic boundary conditions, respectively. The excess entropy is of particular interest in the theory of liquids and glasses. However, often, in the computation of the two-body excess-entropy $s_2$ finite-size effects are overlooked and simulations are treated as if they were in the Grand Canonical ensemble. In this talk, we introduce and validate a finite-size two-body excess-entropy integral equation. Through analytical arguments and computer simulations of prototypical simple liquids, we demonstrate that the excess entropy $s_2$ displays a finite-size scaling with the inverse of the linear size of the simulation box. To valid our expression and given that the self-diffusivity coefficient $D^*$ also exhibits a similar finite-size scaling, we establish that the empirical relation $D^* = A\exp(\alpha s_2)$ also depends on the simulation box size. Extrapolating this relation to the thermodynamic limit, we report values for $A$ and $\alpha$ with excellent agreement with the literature. Finally, we find a power law relation between the scaling coefficients for $D^*(L)$ and $s_2(L)$, suggesting a constant viscosity-to-entropy ratio.

DY 41.6 Thu 10:45 BH-N 128

**Finite-size diffusion coefficients and excess entropy for binary mixtures** — •Maria C. Duenas-Herrera, Mauricio Sevilla, Luis A. Baptista, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Mainz, Germany

A universal relation between transport properties and excess entropy - the difference between a simple liquid's entropy and its ideal gas counterpart at equal density and temperature - has been widely investigated in theoretical, experimental and simulation studies. Similar connections between self-diffusion per component and excess entropy have been proposed for binary mixtures. However, excess-entropy scaling with multi-component diffusion coefficients such as Maxwell-Stefan (MS) or Fick (F) is mainly missing. To contribute to filling this gap, we perform molecular dynamics simulations of prototypical Lennard-Jones binary mixtures from which the excess entropy can be safely approximated to two-body terms. Multi-component diffusion coefficients and two-body excess entropy exhibit explicit and implicit finite-size effects present in conventional computer simulations. By considering finite-size versions of integral equations in statistical mechanics, a robust extrapolation to the thermodynamic limit allows one to establish a consistent scaling behavior of MS and F diffusivities with excess entropy.

**15 min. break**

DY 41.7 Thu 11:15 BH-N 128

**A grand canonical hybrid approach to sample explicit solvent in small solvation shells** — •Mohammad Rahbar and Christopher J. Stein — Technical University of Munich; TUM School of Natural Sciences, Department of Chemistry, Lichtenbergstr. 4, D-85748 Garching, Germany

Solvation effects significantly influence reactions in solution by modifying potential energy surfaces. Treating the solvent with an implicit model often lacks the depth to provide detailed insights into the structure and statistical fluctuations of the solvent. Explicit solvation models are an alternative approach, where both solute and solvent degrees of freedom are explicitly included. However, this method is limited by computational cost already for simulations with a small number of solvent molecules. Therefore, a hybrid approach that combines implicit and explicit methods may offer a more comprehensive understanding. A recurrent challenge in various hybrid methodologies is the lack of inclusion of statistical solvent fluctuation and heavy reliance on chemical intuition for the structure of the solute-solvent microsolvation shell. In our proposed approach, the grand canonical model plays a crucial role in facilitating the transfer of energy and particles between explicit and implicit domains, ensuring agreement with thermodynamic constraints for the simulated system. Free from ad hoc assumptions, our methodology aims to eliminate any nonphysical biases tied to the explicit set of solvent molecules included in the simulation. We construct a framework for accurately sampling solute and solvent configurations at the QM, QM-MM, or purely MM level in a small solvation shell.

DY 41.8 Thu 11:30 BH-N 128

**Analysis of the effects of the entropy source on Monte Carlo simulations** — •Anton Lebedev[1], Olha Ivanyshyn Yaman[1], Annika Möslein[2], Zhanet Zaharieva[2], and Charles Bryant[2] — [1]UKRI-STFC Hartree Centre, Keckwick Ln, Warrington, United Kingdom — [2]Quantum Dice Ltd, Oxford Centre for Innovation, Oxford, United Kingdom

In this contribution we present the benefits of quantum random number generators (QRNGs) for Monte Carlo simulations using select examples from mathematics and physics. We further present the set of statistical tests performed to arrive at this conclusion when comparing QRNGs to (industry-standard) pseudo-random and radio-based random number generators.

From simple Pi estimation to Bayesian model fitting: Monte Carlo applications are ubiquitous. All rely on randomness to sample the solution space, yet analysis of the quality of random number generators is limited. Understanding the effects of the randomness source on MC simulations and leveraging verifiable quantum randomness will yield a reasonable reduction in the number of simulations required to achieve a prescribed uncertainty bound and thereby the amount of compute resources consumed.

Using examples from mathematics and physics, we have analysed the statistically significant differences in simulation outcomes between quantum RNGs, classical hardware RNGs and (parallel) pseudo-random number generators. Tests for statistical significance have been selected based on the amount of underlying assumptions.

DY 41.9 Thu 11:45 BH-N 128

**Population annealing on massively-parallel and distributed compute hardware** — •Denis Gessert[1,2], Wolfhard Janke[1], and Martin Weigel[3] — [1]Institut für Theoretische Physik, Universität Leipzig, 04081 Leipzig — [2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, UK — [3]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Population annealing (PA) is a Monte Carlo (MC) method well suited for problems with a rough free energy landscape such as glassy systems. A PA simulation starts by equilibrating $R$ replicas at an easy-to-sample high temperature. Akin to simulated annealing (SA) of a single system, the replicas are collectively cooled down to an otherwise hard-to-sample low temperature. Unlike in SA, before MC updates at the next lower temperature a selection process is carried out in PA, which makes the algorithm less prone to trapping in metastable states. The population size required to reach equilibrium strongly depends on the "difficulty" of the studied system, with some spin-glass simulations requiring populations of several million replicas. Despite the immediate technical challenge, this opens up an opportunity of achieving a level of parallelism that grows with the difficulty of the task.

Here, we present a simple replica-redistribution protocol for a distributed compute architecture that significantly reduces network traffic as compared to previous approaches, thus improving performance. For small instances, our protocol is only slightly worse than the optimal redistribution protocol found by brute-force. Finally, in some cases a form of speculative execution can be used to hide the network latency.

DY 41.10 Thu 12:00 BH-N 128

**Extrapolation of Rate Functions from Finite-Size Numerical Large-Deviation Simulations** — •Peter Werner and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

When performing large-deviation simulations, a typical question is whether the system at hand follows a *large-deviation principle* [1]. This can be done by checking if the probability distribution of an intensiv system quantity converges for increasing system sizes to a form that possesses a corresponding rate-function. Analytical solutions exist for certain models that allow for comparisons with numerical results [2]. Some special-purpose algorithms, as the *cloning* approach [3], can be used for a direct estimate. However, by using data from arbitrary simulation procedures, the results usually depend heavily on the specific finite-size scaling behaviour of the probability distributions. Here, a numerical procedure is presented that relies on samples obtained from general biased Monte-Carlo simulations [4]. Instead of working with the probability distributions directly, the scaled cumulant-generating function is approximated. From this approximation the *Gärtner-Ellis theorem* is applied to obtain the rate function. Example results are shown for a simple binomial distributed variable and the largest connected component in Erdös-Rényi random graphs.

[1] H. Touchette, Phys. Rep. **478**, 1-69 (2012)
[2] A. K. Hartmann, Eur. Phys. J. Special Topics **226**,567-579 (2017)
[3] E. Hidalgo, JSTAT **2018**, 083211 (2018)
[4] A. K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 41.11 Thu 12:15 BH-N 128

**Calculation of second virial coefficients of convex bodies in $D$-dimensional Euclidean spaces via Brunn-Minkowski theory** — •Markus Kulossa and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

The virial series expands the compressibility factor of imperfect gases in a power series of the particle number density $\varrho$, where the virial coefficient of order $i$ accounts for the contribution of interactions in an $i$-particle cluster to the non-ideal behavior. In the low-density limit, the second virial coefficient is the leading contribution to the departure from ideal gas behavior. For hard particles, the second virial coefficient is the orientationally-averaged mutual excluded volume per particle which is within the Brunn-Minkowski theory analytically accessible via quermassintegrals.

In this talk we present analytical formulations for the second virial coefficient of hard, convex bodies in $D$-dimensional Euclidean spaces $\mathbb{R}^D$ with emphasis on so far unknown expressions for second virial coefficients of uni-axial solids of revolution in $\mathbb{R}^4$. In addition to the effect of the aspect ratio, the detailed influence of the particle shape is analyzed. The effect of the dimensionality $D$ is shown by comparing virial coefficients of 4D objects with their sections in lower-dimensional spaces.

DY 41.12 Thu 12:30 BH-N 128

**Dimensional Phase Transitions in Quantum Gases** — •Philipp Schöneberg[1], Hans-Otto Carmesin[1,2,3], Phil Immanuel Gustke[1], and Jannes Ruder[1] — [1]Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — [2]Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — [3]Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, there occurred a rapid increase of distances usually called 'cosmic inflation'.

We model the objects in the early universe by a quantum gas. We show that there occurred dimensional phase transitions at high density in the early universe. We derive the critical densities. With it we explain the rapid increase of distances usually called 'cosmic inflation'.

Literature: Carmesin, H.-O. (2023): Geometrical and Exact Unification of Spacetime, Gravity and Quanta, Berlin: Verlag Dr. Köster.