DY 5: Poster Session III: Statistical Physics, Complex Fluids and Soft Matter

Time: Tuesday 17:30–19:30 Location: P

DY 5.1 Tue 17:30 P

Correlational entropy by nonlocal quantum kinetic theory — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The nonlocal kinetic equation unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. Large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors [1]. The remaining corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [2]. In this way quantum transport is possible to recast into a quasi-classical picture [3]. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory [4]. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy. For Maxwellian particles a sign change of the latent heat is reported at a universal ratio of scattering length to the thermal De Broglie wavelength. This is interpreted as a change from correlational heating to cooling [5]. [1] Ann. Phys. 294 (2001) 135, [2] Phys. Rev. C 59 (1999) 3052, [3] "'Interacting Systems far from Equilibrium -Quantum Kinetic Theory"' Oxford University Press, (2017) ISBN 9780198797241, [4] Phys. Rev. E 96 (2017) 032106, [5] Phys. Rev. B 97 (2018) 195142

DY 5.2 Tue 17:30 P

Toolbox for quantifying memory in dynamics along reaction coordinates — Alessio Lapolla and •Aljaz Godec — Mathematical bioPhysics Group, Max Planck Institute for Biophysical Chemistry

Memory effects in time series of experimental observables are ubiquitous and may have important consequences for the interpretation of kinetic data. They may even affect the function of biomolecular nanomachines such as enzymes. We propose a set of complementary methods for quantifying conclusively the magnitude and duration of memory in a time series of a reaction coordinate [1]. The toolbox is general, easy to use, and does not rely on any underlying microscopic model. As a proof of concept we apply it to the analysis of memory in the dynamics of the end-to-end distance of the analytically solvable Rouse-polymer model, an experimental time series of extensions of a single DNA hairpin measured by optical tweezers, and the fraction of native contacts in a small protein probed by atomistic molecular dynamics simulations.

[1] A. Lapolla and A. Godec, Phys. Rev. Research 3, L022018 (2021)

DY 5.3 Tue 17:30 P

Depinning of confined colloidal dispersions under oscillatory shear — •Marcel Hülsberg and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Strongly confined colloidal dispersions under shear exhibit a variety of dynamical phenomena, including a depinning transition similar to single particles that are driven over a periodic substrate potential [1].

Here, we investigate the depinning behavior of these systems under pure oscillatory shearing with shear rate $\dot\gamma(t) = \dot\gamma_0 \cos(\omega t)$, as it is a common scenario in rheological experiments [2].

The colloids' depinning behavior is assessed from a microscopic level based on particle trajectories, which are obtained from overdamped Brownian Dynamics simulations. The numerical approach is complemented by an analytic one based on a single-particle model in the limit of weak driving.

Investigating a broad spectrum of shear rate amplitudes $\dot\gamma_0$ and frequencies ω, we observe complete pinning as well as temporary depinning behaviour. We discover that temporary depinning occurs for shear rate amplitudes above a frequency-dependent critical amplitude $\dot\gamma_0^{\mathrm{crit}}(\omega)$, for which we attain a functional expression. This allows us to identify the dominant system-intrinsic time scale that dictates the scaling behavior of $\dot\gamma_0^{\mathrm{crit}}$ with driving frequency ω.

Finally, we discuss the connection between depinning and structural changes in the system.

[1] S. Gerloff and S.H.L. Klapp, Phys. Rev. E **94**(6), 062605 (2016)
[2] J.M. Brader, et al., Phys. Rev. E **82**(6), 061401 (2010)

DY 5.4 Tue 17:30 P

Emergence of collective motion in two-dimensional colloidal systems with delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback (dFB) in colloidal systems has become an active and promising field of study [1,2,3], key topics being history dependence and the manipulation of transport properties. Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen (WCA) potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential (cf. [1]), that depends on the difference of the particle position at the current time, $\mathbf{r}_i(t)$ and the particle position at an earlier time, $\mathbf{r}_i(t-\tau_{\mathrm{delay}})$. We observe the emergence of collective motion characterized by a nonzero mean velocity. After quantitatively studying this phenomenon, we also provide a possible explanation combining single-particle and mean-field-like effects.

[1] S. Tarama, S. U. Egelhaaf, and H. Löwen, Physical Review E **100**, 022609 (2019)
[2] R. Gernert and S. H. L. Klapp, Physical Review E **92**, 022132 (2015)
[3] S. A. M. Loos, and S. H. L. Klapp, Scientific Reports **9**, 2491 (2019)

DY 5.5 Tue 17:30 P

Brownian magneto-gyrator as a tunable microengine — •Iman Abdoli[1], René Wittmann[2], Joseph Michael Brader[3], Jens-Uwe Sommer[1,4], Hartmut Löwen[2], and Abhinav Sharma[1,4] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Dresden, 01069, Germany — [2]Institut für Theoretische Physik II, Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, 40225, Germany — [3]Department de Physique, Université de Fribourg, CH-1700 Fribourg, Switzerland — [4]Technische Universität Dresden, Institut für Theoretische Physik, Dresden, 01069, Germany

A Brownian particle performs gyrating motion around a potential energy minimum when subjected to thermal noises from two different heat baths. Here, we propose a magneto-gyrator made of a single charged Brownian particle that is steered by an external magnetic field. Key properties, such as the direction of gyration, the torque exerted by the engine on the confining potential and the maximum power delivered by the microengine can be tuned by varying the strength and direction of the applied magnetic field. Further tunability is obtained with a potential that couples the spatial degrees of freedom. We show that in this generic scenario, the microengine can be stalled and even reversed by the magnetic field. Finally, we highlight a property of the magneto-gyrator that has no counterpart in the overdamped approximation–the heat loss from the hot to cold bath requires explicit knowledge of the mass of the particle. Consequently, the efficiency of the microengine is mass-dependent even in the overdamped limit.

DY 5.6 Tue 17:30 P

Broadband frequency filters with quantum dot chains — •Tilmann Ehrlich[1] and Gernot Schaller[1,2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Two-terminal electronic transport systems with a rectangular transmission can violate standard thermodynamic uncertainty relations. This is possible beyond the linear response regime and for parameters that are not accessible with rate equations obeying detailed-balance. Looser bounds originating from fluctuation theorem symmetries alone remain respected. We demonstrate that optimal finite-sized quantum dot chains can implement rectangular transmission functions with high accuracy and discuss the resulting violations of standard thermodynamic uncertainty relations as well as heat engine performance.

[1] arXiv:2103.04322, to appear in PRB

DY 5.7 Tue 17:30 P

Cosmological and Elementary Particles Explained by Phase Transitions Derived by Quantum Gravity — •Hans-Otto

Carmesin — Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, the density was very high. As a consequence, there occurred gravitational instabilities and corresponding dimensional phase transitions, see Carmesin, Hans-Otto (March 2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin, Dr. Köster Verlag. These transitions are very robust, as they occur in three very different physical systems.

Based on the quantum states corresponding to these dimensional transitions, we derive many excitation modes that include the formation of neutrinos, of the Higgs boson, of the quanta of dark energy, and of many novel elementary particles, see Carmesin, Hans-Otto (August 2021): Cosmological and Elementary Particles Explained by Quantum Gravity. Berlin, Dr. Köster Verlag. These particles range form the Planck scale to the lightest particles, and so they solve the hierarchy problem of particle physics.

All results are derived by quantum gravity and are in precise accordance with observation. I emphasize that the only numerical input used in my theory is the present day time after Big Bang combined with the universal constants G, c, k_B and h.

DY 5.8 Tue 17:30 P

Dimensional Phase Transitions of a Bose Gas in the Early Universe — •Paul Sawitzki[1] and Hans-Otto Carmesin[1,2,3] — [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, the density was very high. As a consequence, there occurred gravitational instabilities and corresponding dimensional phase transitions, see Carmesin, Hans-Otto (March 2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin, Dr. Köster Verlag. These transitions are very robust, as they occur in three very different physical systems. Here we derive these transitions for the case of a Bose gas.

These transitions are essential for various fields of cosmology, including the so-called era of 'cosmic inflation' and the solution of the horizon problem.

All results are derived by quantum gravity and are in precise accordance with observation. We emphasize that the only numerical input used in the theory is the present day time after Big Bang combined with the universal constants G, c, k_B and h.

DY 5.9 Tue 17:30 P

Diagrammatic expansion of the two-point effective action around non-Gaussian theories — •Tobias Kühn and Frédéric van Wijland — Laboratoire Matière et Systèmes Complexes, Université de Paris

Consider a many-body problem, such as one involving interacting spins, particles or the time series of a random signal, of which we know the corresponding one- and two-point correlation functions. We suppose that the distribution of the spin values (or particle positions,...) is written in a Boltzmann form with a Hamiltonian possessing one- and two-body interactions only. How does one choose the corresponding couplings so that the distribution generates the prescribed statistics? This so-called inverse problem is conveniently described by the second Legendre transform of the cumulant-generating function, the two-point effective action, whose arguments are means and correlations. The couplings we seek for are then explicitly given by its derivatives. Weak correlation approximations have been proven useful to compute the two-point effective action (Sessak & Monasson 2009). As long as the one-body problem is described by independent Gaussian distributions, they can be routinely derived using diagrammatic methods dating back to Feynman, Luttinger and Ward. Here we explain how similar diagrammatics can be extended to the case in which the one-body problem is not of a Gaussian nature. We discuss how this can prove useful in inference problems pertaining to neuroscience and other complex systems. Another possible application is the derivation of mean-field theories self-consistently taking into account pairwise correlations.

DY 5.10 Tue 17:30 P

Charged Liquid Bridges — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A new solution of a charged catenary is presented which allows to determine the static and dynamical stability conditions where charged liquid bridges are possible. The creeping height, the bridge radius and length as well as the shape of the bridge is calculated showing an asymmetric profile in agreement with observations. The flow profile is calculated from the Navier Stokes equation leading to a mean velocity which combines charge transport with neutral mass flow and which describes recent experiments on water bridges. The velocity profile in a water bridge is reanalyzed. Assuming hypothetically that the bulk charge has a radial distribution, a surface potential is formed that is analogous to the Zeta potential. The Navier*Stokes equation is solved, neglecting the convective term; then, analytically and for special field and potential ranges, a sign change of the total mass flow is reported caused by the radial charge distribution. [Water 9 (2017) 353, Phys. Rev. E 86 (2012) 026302, errata Phys. Rev. 86 (2013) 069904, AIP Advances 2 (2012) 022146-1-6]

DY 5.11 Tue 17:30 P

Ornstein-Zernike relation in hypergraphs — •Christian Faber[1,2,3], Till Kranz[2,3], and Matthias Sperl[3,2] — [1]Jülich Supercomputing Centre, FZ Jülich — [2]Institut für Theoretische Physik, Uni Köln — [3]Institut für Materialphysik im Weltraum, DLR Köln

The pair correlation function is an important input to describe equilibrium phase transitions and the glass transitions [1]. An Ornstein-Zernike relation can be used to represent the pair correlation function in a form that is easy to approximate and that allows an intuitive representation in terms of graphs [2]. However, this graphical representation is limited to pairwise interactions between particles and recent analyses show that some systems, such as foams, cannot be adequately represented with pair interactions [3]. To be able to specify a meaningful Ornstein-Zernike relation for such systems, we have started from scratch and have introduced hypergraphs for multi-body interactions. With these we are able to represent the Ornstein-Zernike relation for multi-body interactions and to give a graphical meaning to the individual terms. We will discuss the similarities and differences between the relation for pair- and for multi-body interactions.

[1] W. Götze, *Zeitschrift f. Physik B Condensed Matter* **60**, 2 (1985).
[2] M. Wortis, "Linked Cluster Expansion" in *Phase Transitions and Critical Phenomena*, C. Domb, M.S. Green, Eds. (Academic Press, London, 1974), vol. 3.
[3] G. Ginot, R. Höhler, S. Mariot, A. Kraynik, W. Drenckhan, *Soft Matter* **15.22**, 4570-4582 (2019).

DY 5.12 Tue 17:30 P

Phase behaviour of a generalized chiral Lebwohl-Lasher model — •Anja Kuhnhold and Philipp Elsässer — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

The Lebwohl-Lasher (LL) model is a simple model to study the isotropic-nematic (IN) transition of liquid-crystalline systems. Particles are described by unit vectors that sit on a simple cubic lattice and only interact with nearest neighbours; the interaction potential has a minimum for parallel orientation of the particles' axes, which drives the IN transition.

Fish and Vink generalized the LL model so that the sharpness of the potential can be tuned and with that the type of phase transition in the 2D limit [1]. Memmer et al. added a chiral interaction to the LL model. They studied the resulting cholesteric phase (where the orientation of particles is parallel within a layer but is rotated between layers) and its behaviour when confined between aligning surfaces [2]. We combine both extensions to the generalized chiral Lebwohl-Lasher model and study the isotropic-cholesteric transition depending on the sharpness parameter, the chirality, and the dimensionality of the system. We use a Wang-Landau Monte-Carlo method to simulate the system and apply finite-size scaling to identify the type of phase transitions.

[1] J.M. Fish, R.L.C. Vink, PRE **81**, 021705 (2010).
[2] R. Memmer, O. Fliegans, PCCP **5**, 558 (2003).

DY 5.13 Tue 17:30 P

Microsecond XPCS on soft matter probed at the European XFEL — •Francesco Dallari and Felix Lehmkühler — Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

Many soft-matter systems are composed of nanoparticles or macromolecules dispersed in water. The characteristic time at the relevant length-scales of few nanometers falls therefore in the (sub)microsecond time-scales, making the measurement of the dynamical properties for these system an extremely challenging (often impossible) task at third generation synchrotron light sources. With the recent development of hard X-ray free electron lasers (XFELs) and fourth generation light sources, time-resolved experiments in this time- and length-scale regimes have become accessible. Here we present the first results on prototypical charge-stabilized silica nanoparticles dispersed in water both in diluted [1] and concentrated [2] systems. Tuning the pulse fluence we are able to probe and describe with thermodynamical models the diffusion properties in stationary systems and in systems driven by the XFEL pulses.

Bibliography:

[1] F. Lehmkühler, F. Dallari, A. Jain, et al. (2020). PNAS, 117, 24110-24116. https://doi.org/10.1073/pnas.2003337117

[2] F. Dallari, ,A. Jain, F. Lehmkühler, et al. (2021). IUCrJ 8, https://doi.org/10.1107/S2052252521006333.

DY 5.14 Tue 17:30 P

Efficient Event-Driven Simulation of the Bubbling Instability in a Fluidised Bed — Raphael Biertz[1], •Till Kranz[1,2], and Matthias Sperl[2,1] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

Two-phase flows, comprised of granular particles and an interstitial molecular fluid occur in many places in nature and industry. The prototypical setup for this kind of complex fluid is a fluidised bed. At sufficient fluidisation flow rates, the particulate phase displays a bubbling instability with close packed and very dilute regions [1].

While pure granular fluids are efficiently simulated by event-driven molecular dynamics algorithms, the two-phase flow problem is still a numerical challenge. Here, we discuss that an implicit model of the fluidising fluid in combination with a event-driven approach for the particles [2] can faithfully capture the bubbling instability [3].

[1] Jackson, R., *The Dynamics of Fluidized Particles*, Cambridge University Press, 2000

[2] Fiege, A., Zippelius, A., J. Phys.: Conf. Ser. **759**, 012001 (2016)

[3] Biertz, R., Sperl, M., Kranz, W. T., in preparation

DY 5.15 Tue 17:30 P

Topological optimization of microfluidic Tesla valves for applications with low Reynold numbers — •Sebastian Bohm[1], Hai Binh Phi[2], Ayaka Moriyama[3], and Erich Runge[1] — [1]TU Ilmenau, FG Theoretische Physik I, DE — [2]TU Ilmenau, FG Mikrosystemtechnik, DE — [3]Carleton College, Physics Department, USA

Passive Tesla valves represent a promising method for rectifying flows in microfluidic systems because no moving parts are needed. The efficiency of the valves is characterised by the diodicity which can be defined as the pressure drop ratio of the forward and the reverse flow direction. To obtain efficient valve designs, topological optimization has proven to be a particularly suitable method [1]. The challenge is the dependency of the diodicity on the Reynolds number. Normally, the valves are only efficient at Reynolds numbers much greater than 100. In microfluidics, Reynolds numbers are usually very low, which hitherto limits the applicability of Tesla valves. Therefore a novel approach for the topological optimization of valves that work at very small Reynolds numbers is presented: To ensure that the optimization yields meaningful designs, a customized objective function is introduced and a multi-stage optimization procedure is used. In addition, a method is presented to optimize the diodicity over a given range of Reynolds numbers simultaneously. The resulting valves achieve a diodicity of up to 2 already at Reynolds numbers smaller than 20. The simulated predictions are in close agreement to experimental results.

[1] S. Lin et al., *Topology Optimization of Fixed-Geometry Fluid Diodes*, J. Mech. Des., 137 **(8)**, (2015)